Genehmigte Dissertation der Fakultät für Physik der Universität Duisburg-Essen zur Erlangung des Grades eines Doktors der Naturwissenschaften (Dr. rer. nat.)

Pointer state dynamics of dissipative quantum systems

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geboren am 15. September 1986 in Berlin

Duisburg, den 24. Juni 2016

Tag der mündlichen Prüfung: 10. Oktober 2016
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Zusammenfassung

In der vorliegenden Arbeit identifiziere ich die Zeigerzustände der quantenbrownschen Bewegung als rotierte gaußsche Zustände im Phasenraum. Mithilfe des Zeigerzustandsunravelings, ein bestimmtes stückweise deterministisches Unraveling, leite ich die Trajektorien der Orts- und Impulserwartungswerte der Zeigerzustände ab. Es stellt sich heraus, dass diese durch einen Diffusionsprozess im Phasenraum beschreibbar sind, und dass sie im semiklassischen Grenzfall die Langevingleichung der klassischen brownschen Bewegung ergeben. Für Stoßdekohärenz, den nichtdissipativen Grenzfall der quantenlinearen Boltzmanngleichung, welcher die Dynamik eines in einem idealen Gas eingetauchten Markerteilchens beschreibt, untersuche ich die Breite der Zeigerzustände und erweitere dabei frühere Ergebnisse auf mehr als eine Dimension. Als entscheidender Unterschied folgt, dass in diesem Fall die Zeigerzustände nicht für alle Parameterbereiche existieren. Durch eine Entwicklung der Lindbladoperatoren der quantenlinearen Boltzmanngleichung leite ich eine neue Lindbladmastergleichung her, dissipative Stoßdekohärenz, die ein Dekohärenzverhalten ähnlich dem der Stoßdekohärenz hat, und darüberhinaus auch Reibungs- und Diffusionseffekte enthält. Außerdem zeigt sie solitonartige Lösungen, welche Kandidaten für die Zeigerzustände darstellen.

Abstract

In the present work, I identify the pointer states of quantum Brownian motion as rotated Gaussian states in phase space. By means of a particular piecewise deterministic unraveling, the pointer state unraveling, I determine the trajectories of the position and momentum expectation of the pointer states. They turn out to be described by a diffusion process in phase space and, in the semiclassical limit, they turn into the Langevin equation of classical Brownian motion. For collisional decoherence, the non-dissipative limit of the quantum linear Boltzmann equation, which describes the dynamics of a marker particle in an ideal gaseous environment, I examine the width of the pointer states and thereby extend previous results to more than one dimension. Crucially, it follows that pointer states do not exist for all parameter values in that case. By expanding the Lindblad operators of the quantum linear Boltzmann equation, I derive a new Lindblad master equation, dissipative collisional decoherence, which shows a decoherence behavior similar to that of collisional decoherence and also incorporates frictional as well as diffusion effects. Moreover this equation exhibits soliton-like solutions as candidates for the pointer states.

Danksagung

Zuvorderst möchte ich der gesamten Arbeitsgruppe für die schöne Zeit and der Uni Duisburg danken. Dafür, dass wir wohl kaum ein Thema beim Mittagstisch ausgelassen haben und dass wir gemeinsam viel Spaß und interessante Diskussionen hatten. Möglich wird dies durch Klaus, der eine angenehme Arbeitsatmosphäre schafft und genügend Freiraum für die eigene Entfaltung lässt. Maßgeblich durch ihn sind wir beispielsweise motiviert worden neben der gemeinsamen Arbeit auch gemeinsam zu Grillen. Natürlich war es auch Klaus, der es mir ermöglichte, mich überhaupt mehrere Jahre intensiv mit solch interessanter Physik zu beschäftigen und mich wissenschaftlich weiterzubilden. Für die viele Geduld und dafür, dass er immer ein offenes Ohr und eine offene Tür für fachliche (und sonstige) Diskussionen hat, möchte ich Klaus besonders danken.
Den Menschen, die mein Leben in Duisburg außerhalb der Uni mitgestaltet haben, dies sind hauptsächlich diejenigen, mit denen ich zusammen gewohnt habe und mit denen ich Capoeira trainieren durfte, möchte ich auch herzlich danken. Dafür, dass auch wir soviel Spaß hatten und dass wir gemeinsam voneinander lernen konnten. Sie haben mir den nötigen nicht-physikalischen Ausgleich zur Arbeit beschert und damit, da bin sicher, zum Gelingen meiner Promotion sehr viel beigetragen. Meinen Eltern schließlich möchte ich dafür danken, dass sie mich durchgehend in meinen Interessen unterstützen und mir dadurch die Möglichkeiten geben, meine eigenen Wege zu finden und zu gehen. Auch dieser Freiraum hat mir beim fachlichen aber besonders beim persönlichen Fortschreiten hier in Duisburg sehr geholfen.

Contents

1. Introduction

Motivation

Quantum theory lies at the heart of our understanding of atomic and sub-atomic physics. Up to now, it has withstood all experimental tests, for instance, matter-wave interference experiments, which challenge the superposition principle for large molecules with masses as high as several thousand atomic mass units [1–4], or high accuracy loophole-free tests of Bell's inequalities [5–7]. The wide applicability of quantum theory leads one to the expectation that it is also valid at macroscopic scales, however, there is still no complete consensus about its relation to classical physics. Quantum phenomena such as superposition states seem quite incompatible with the reality one usually perceives. It is therefore natural to ask for a framework that incorporates quantum mechanics and allows for an explanation of classicality.

One possible route for explaining classicality might be to modify the Schrödinger equation by a stochastic term that has nearly no effect on microscopic scales but leads to localization for macroscopic superpositions [8, 9]. It enables one to consistently describe quantum dynamics, measurements, and emergent classical properties. On the other hand, one can approach the quantum-to-classical transition from within the standard quantum mechanics realm, using a non-modified Schrödinger equation. In this context, it has to be realized that most quantum systems are not isolated but coupled to their environments. The quantum description of the combined system and environment and the subsequent restriction to the reduced system state can lead to approximate equations for the system density operator, i.e. to master equations that, generically, show *decoherence*. This has proven a viable concept for the explanation of classicality [10–14], where decoherence means a reduction of the system state coherences, which is mediated by the practically unobservable environmental degrees of freedom.

The so-called *pointer states* play an important role at this stage, for they build preferred states, which do not decohere [11, 15–17]. The name pointer states derives from their behavior being similar to that of a pointer of a measuring apparatus: If a quantum system is in an eigenstate of the observable one wants to measure with the apparatus, then, upon measurement, the apparatus' pointer will turn to the appropriate value on the dial and stay there. On the other hand, if the system is in a superposition of two nondegenerate eigenstates, the unitary evolution would prescribe the pointer to be in a superposition of the two corresponding eigenvalues on the dial. However, one finds that the pointer goes either to one or the other position with probabilities determined from the superposition state via Born's rule.

There have been different suggestions how to obtain the set of pointer states, among

them the predictability sieve, which requires that the pointer states should be the least entropy producing states of the system [18, 19]. Here, I follow another approach, in which the pointer states are identified as soliton-like solutions of a nonlinear equation associated with the master equation. This nonlinear pointer state equation can be obtained heuristically by identifying the pure state evolution closest to the master equation evolution [20, 21]. To draw a precise connection between the pointer state equation and the master equation a so-called *unraveling* is used [21]. Conceptually, it builds on the similar correspondence between a Fokker-Planck equation and a Langevin equation in classical systems. The former is the equation of motion for the distribution function, whereas the latter is a stochastic differential equation for the accompanied ensemble of phase space trajectories. In this sense, instead of using the density matrix and its master equation evolution, one applies an unraveling that describes an ensemble of pure states, the quantum trajectories, via a stochastic differential equation.

With the unraveling of the master equation at hand, the quantum-to-classical transition is pictured by a description of the master equation evolution of the open quantum system by means of an ensemble of stochastically moving pointer states. Going further into the classical regime, the pointer states in each quantum trajectory get thinner, i.e. more localized, and eventually may be identified with points in phase space. Additionally, and equally important, the trajectories of the pointer states turn into those one expects from an analogous classical system. In this way, the unraveling with the help of pointer states also provides a method to characterize the solutions of complicated quantum master equations.

It should be emphasized here that decoherence theory, though it is able to explain the disappearance of macroscopic superpositions, does not select one particular member of the arising mixture of states. Thus, it cannot explain any wave function collapse during quantum measurements and therefore it does not solve the measurement problem [12, 22–24].

Scope of the thesis

In this thesis, I advocate the use of the pointer state unraveling to analyze the quantum-to-classical transition of dissipative particle motion. In general, the dynamics of a test particle immersed in an ideal gaseous environment can be described by the quantum linear Boltzmann equation [25]. From this equation, one can derive several limiting cases, where particular interest is devoted to the quantum Brownian limit. This limit is exhibited for a massive test particle in a state close to equilibrium, which implies that the particle is exposed to small kicks. In one form or another, quantum Brownian motion already has a long history and serves as a paradigmatic model for dissipative quantum dynamics [26–34]. Moreover, its classical counterpart, whose theoretical description started at the beginning of the 20^{th} century, constituted a breakthrough for atomism [35, 36]. Among the several formulations of quantum Brownian motion, I mention the Caldeira–Leggett master equation [26] as a first successful attempt to treat dissipative quantum dynamics. It is very similar to the quantum Brownian motion master equation

I discuss here; their difference lying in the fact that the former is not completely positive and thus does not exhibit Lindblad form.

In particular, I characterize the pointer states of quantum Brownian motion as Gaussian states that are rotated in phase space and get more and more localized in the semiclassical limit. Furthermore, I apply the pointer state unraveling to investigate the gradual emergence of the pointer states and their dynamics. This includes at first that superpositions of pointer states decohere into a mixture with the appropriate probabilities as given by the Born rule. Then, I show how each quantum trajectory describes a pointer state that moves on a diffusion-like trajectory in phase space. In the semiclassical limit, this trajectory turns into the one that is expected from classical Brownian motion. This problem is especially interesting as the expected classical trajectories are stochastic in nature and their derivation requires a thorough analysis of the interplay between the deterministic and the stochastic part of the quantum trajectory.

The pointer state unraveling, which I apply in this work, has already been used by Busse and Hornberger [37–39] to analyze the collisional decoherence master equation. This master equation can be obtained as the non-dissipative limit of the quantum linear Boltzmann equation [25, 40], which is exhibited for an infinite mass of the marker particle. Busse and Hornberger find that the pointer states of one-dimensional collisional decoherence are exponentially localized and move on deterministic trajectories according to Newton's laws. Here, I extend this discussion to more than one dimension and derive an approximation method via Gaussian states that allows for the calculation of the pointer states' width. It follows that pointer states in two and three dimensions only exist for certain parameter values.

A further step in characterizing the dynamics of the quantum linear Boltzmann equation is then done by deriving a master equation in a regime that extends both the quantum Brownian motion limit and the collisional decoherence limit. For this, a Taylor expansion of the Lindblad operators of the quantum linear Boltzmann equation to first order in the mass ratio between the environmental gas particles and the marker particle is performed. Notice that the expansion to zeroth order gives the non-dissipative limit of collisional decoherence. I call the equation the dissipative collisional decoherence master equation and characterize it by showing its decoherence properties and derive and solve equations of motion for the first moments and variances in phase space, which clearly show friction and diffusion effects. An analysis of the existence of pointer states completes this final part of the thesis.

Structure of the thesis

The first two chapters serve as an introduction of important techniques that I need throughout this work and may be skipped by those familiar with the topics. Specifically, in Chapter 2, I discuss the relevant classical stochastic processes and introduce the concept of stochastic differential equations, for both diffusive and piecewise deterministic processes. Particular interest is devoted to the description of a diffusion process in phase space, because it is important for characterizing the pointer state trajectories of

quantum Brownian motion. Moreover it includes, as a special case, classical Brownian motion, which is the expected classical counterpart of quantum Brownian motion. In the following Chapter 3, I present the quantum mechanical concepts, which are needed later on. They include Markovian open quantum systems and their description by a Lindblad master equation. Furthermore, the relevant master equations are introduced and discussed. Finally, I introduce the concept of pointer states and their connection to a Lindblad master equation via the pointer state unraveling.

The Gaussian pointer states of quantum Brownian motion as well as their dynamics are derived in Chapter 4. I show that superpositions of localized states decohere into a mixture of pointer states, with probabilities according to Born's rule. The interplay of the stochastic and the deterministic part in the stochastic equation of motion for the quantum trajectories then allows me to describe the pointer state motion as a diffusive stochastic trajectory, which turns into the one of classical Brownian motion in the semiclassical limit.

In the subsequent Chapter 5, I concentrate on aspects of the collisional decoherence model, which are not discussed in Refs. [37–39]. Namely, I discuss the pointer states of collisional decoherence in two and three dimensions. While their shape remains unchanged in comparison with the one-dimensional treatment, they are exponentially localized, there are substantial differences regarding the width of the pointer states in more than one dimension. For that, a localization model based on the approximation of the pointer states by Gaussian states is developed and applied.

Finally, in Chapter 6, I derive a dissipative Lindblad master equation from the quantum linear Boltzmann equation in a limit that goes beyond both the collisional decoherence and the quantum Brownian motion limit, the dissipative collisional decoherence master equation. It shows decoherence in position quite similar to that of collisional decoherence. In addition to that, one observes friction effects from the derivation and solution of the equations of motion for the position and momentum expectations. The equations of motion for the variances of the master equation lead to dissipative behavior. As the last step, a discussion on the existence of pointer states is done with the help of the Gaussian localization model, which I developed and already applied to the collisional decoherence case. In Chapter 7, I present my conclusions.

2. Classical stochastic processes

This chapter shall give a brief introduction into Markovian stochastic processes because of their importance for many aspects in this thesis. After fixing some notation, I start with a discussion of the differential Chapman–Kolmogorov equation for it shows the two essential types of stochastic motion that are used within this thesis.

Afterwards, I focus on continuous stochastic processes based on the Wiener process and define the corresponding stochastic differential equations. As examples, a diffusion in phase space and, as a special case, classical Brownian motion are presented. They both will be important in Chapter 4 to identify the trajectories of the semiclassical counterpart of quantum Brownian motion.

In the last section, I concentrate on stochastic jump differential equations, which are piecewise deterministic processes and are based on the Poisson process. Their extension to the quantum case in Section 3.7 gives rise to the quantum trajectories of quantum Brownian motion. Here, an important example is given by the random walk and its diffusive limit, which yields a Wiener-based process as a certain limit of a Poisson-based process. As a crucial step in Chapter 4, the pointer state's trajectories of quantum Brownian motion are obtained via such a diffusive limit.

Introductions into the topic can be found, for instance, in Refs. [37, 41–43].

2.1. Basic concepts

Stochastic processes A stochastic process is defined by a time-dependent random variable $\boldsymbol{X}(t)$ that has the value $\boldsymbol{x}_0$ at the initial time t_0 and takes the values $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots,$ $\boldsymbol{x}_n$ at the ordered times $t_1 < t_2 < \cdots < t_n$. The $\boldsymbol{x}_i$ define a trajectory that is, by definition, stochastic and represents one possible realization of the stochastic process. The temporal evolution of these trajectories is governed by stochastic differential equations, which are introduced later in this chapter. Before that, I want to give an understanding of the description of stochastic processes on basis of their ensemble properties, which is done with the help of a *probability density function* $p(\boldsymbol{x}, t)$. It is defined as the probability of $\boldsymbol{X}(t)$ to be in the interval $[\boldsymbol{x}, \boldsymbol{x} + \mathrm{d}\boldsymbol{x}]$ at a time t,

$$\mathrm{Prob}\left(\boldsymbol{x} \leq \boldsymbol{X}(t) < \boldsymbol{x} + \mathrm{d}\boldsymbol{x}\right) \equiv p(\boldsymbol{x}, t)\mathrm{d}\boldsymbol{x}. \tag{2.1}$$

In general, $p(\boldsymbol{x}, t)$ depends on the initial state of the process, described by the distribution $p(\boldsymbol{x}_0, t_0)$, which renders it convenient to introduce the *joint probability density* $p(\boldsymbol{x}_1, t_1; \boldsymbol{x}_0, t_0)$; it stands for the probability to be at $\boldsymbol{x}_0$ at t_0 *and* at $\boldsymbol{x}_1$ at t_1. From these definitions, one gets a whole family of joint probability densities up to the final

time t_n,

$$\begin{gathered} p(\boldsymbol{x}_0, t_0), \\ p(\boldsymbol{x}_1, t_1; \boldsymbol{x}_0, t_0), \\ \dots, \\ p(\boldsymbol{x}_n, t_n; \dots; \boldsymbol{x}_0, t_0). \end{gathered} \tag{2.2}$$

To examine the possible evolution of a stochastic process provided a certain sequence $\boldsymbol{x}_n, \dots, \boldsymbol{x}_0$, instead of using the joint probabilities one introduces a *conditional probability density*, where $p(B|A)$ is the probability for event B to occur conditioned on the fact that event A occured, i.e. $p(B;A) = p(B|A)p(A)$. One then gets from Eqs. (2.2)

$$p(\boldsymbol{x}_{n+1}, t_{n+1}; \dots; \boldsymbol{x}_0, t_0) = p(\boldsymbol{x}_{n+1}, t_{n+1}|\boldsymbol{x}_n, t_n; \dots; \boldsymbol{x}_0, t_0) p(\boldsymbol{x}_n, t_n; \dots; \boldsymbol{x}_0, t_0). \tag{2.3}$$

Markov processes As the last line of Eqs. (2.2) implies, the stochastic process at t_n depends on all former times $t < t_n$, i.e. on its whole history. This situation simplifies a lot if only the most recent value at time t_{n-1} were important. With the help of conditional probability densities, one writes this condition of a "short memory" as

$$p(\boldsymbol{x}_n, t_n|\boldsymbol{x}_{n-1}, t_{n-1}; \dots; \boldsymbol{x}_0, t_0) = p(\boldsymbol{x}_n, t_n|\boldsymbol{x}_{n-1}, t_{n-1}), \tag{2.4}$$

which is called the *Markov condition*. Thus, knowing $p(\boldsymbol{x}_n, t_n|\boldsymbol{x}_{n-1}, t_{n-1})$, the so-called *propagator*, for all times together with the initial condition $p(\boldsymbol{x}_0, t_0)$ already captures the whole process,

$$p(\boldsymbol{x}_n, t_n; \dots; \boldsymbol{x}_0, t_0) = p(\boldsymbol{x}_n, t_n|\boldsymbol{x}_{n-1}, t_{n-1}) \dots p(\boldsymbol{x}_1, t_1|\boldsymbol{x}_0, t_0) p(\boldsymbol{x}_0, t_0). \tag{2.5}$$

An equation for the propagator is then derived by using the Markov condition and $p(A) = \int \mathrm{d}B\, p\,(A;B)$,

$$p(\boldsymbol{x}_3, t_3|\boldsymbol{x}_1, t_1) = \int \mathrm{d}\boldsymbol{x}_2 p(\boldsymbol{x}_3, t_3|\boldsymbol{x}_2, t_2) p(\boldsymbol{x}_2, t_2|\boldsymbol{x}_1, t_1). \tag{2.6}$$

It is known as the *Chapman–Kolmogorov equation* [44].

Stochastic independence Two events A_1 and A_2 are said to be *stochastically independent* if and only if the probability of their joint occurence factorizes,

$$\mathrm{Prob}\,(A_1 \text{ and } A_2) = \mathrm{Prob}\,(A_1)\,\mathrm{Prob}\,(A_2)\,. \tag{2.7}$$

For three events A_1 , A_2, and A_3 to be stochastically independent, analogous factorization properties have to hold for the four possible joint probabilities

$$\begin{gathered} \mathrm{Prob}\,(A_1 \text{ and } A_2)\,, \\ \mathrm{Prob}\,(A_2 \text{ and } A_3)\,, \\ \mathrm{Prob}\,(A_1 \text{ and } A_3)\,, \\ \mathrm{Prob}(A_1 \text{ and } A_2 \text{ and } A_3). \end{gathered} \tag{2.8}$$

The extension to more than three stochastic processes is done accordingly.

Ensemble averages The ensemble average of an arbitrary function $f(\boldsymbol{X}(t))$ of the stochastic process is defined with the help of its probability density by the integral

$$\mathrm{E}\left[f\left(\boldsymbol{X}(t)\right)\right] \equiv \int f(\boldsymbol{x}) p(\boldsymbol{x}, t|\boldsymbol{x}_0, t_0) \mathrm{d}\boldsymbol{x}. \tag{2.9}$$

For instance, in the one-dimensional case the mean value reads

$$\mathrm{E}\left[X(t)\right] = \int x p(x, t|x_0, t_0) \mathrm{d}x \tag{2.10}$$

and the corresponding variance is given by

$$\mathrm{Var}\left[X(t)\right] = \mathrm{E}\left[X(t)^2\right] - \left(\mathrm{E}\left[X(t)\right]\right)^2. \tag{2.11}$$

2.2. Discussion of the Chapman–Kolmogorov equation

For actual calculations it is often more convenient to consider the *differential Chapman–Kolmogorov equation* that is derived from its integral form Eq. (2.6) [41]

$$\begin{aligned}\frac{\partial}{\partial t} p(\boldsymbol{z}, t|\boldsymbol{x}, t') = &- \sum_i \frac{\partial}{\partial z_i}\left[A_i(\boldsymbol{z}, t) p(\boldsymbol{z}, t|\boldsymbol{x}, t')\right] + \frac{1}{2}\sum_{i,j} \frac{\partial^2}{\partial z_i \partial z_j}\left[D_{ij}(\boldsymbol{z}, t) p(\boldsymbol{z}, t|\boldsymbol{x}, t')\right] \\ &+ \int \mathrm{d}\boldsymbol{y}\left[W(\boldsymbol{z}|\boldsymbol{y}, t) p(\boldsymbol{y}, t|\boldsymbol{x}, t') - W(\boldsymbol{y}|\boldsymbol{z}, t) p(\boldsymbol{z}, t|\boldsymbol{x}, t')\right], \end{aligned} \tag{2.12}$$

with the drift vector $\boldsymbol{A}(\boldsymbol{z}, t)$, the positive semidefinite diffusion matrix $\mathsf{D}(\boldsymbol{z}, t)$, and the non-negative transition rate $W(\boldsymbol{z}|\boldsymbol{y}, t)$. The different terms in Eq. (2.12) give rise to a variety of forms of motion, such as drift, diffusion, and jump processes, which are, in general, superimposed. For a better understanding of the action of each term, I consider each of them separately and also discuss some properties of the corresponding trajectories of each kind of motion.

2.2.1. Deterministic motion

If $\mathsf{D}(\boldsymbol{z}, t)$ and $W(\boldsymbol{z}|\boldsymbol{y}, t)$ vanish, the equation ensuing from (2.12) describes a deterministic motion where each trajectory is governed by the ordinary differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}(t) = \boldsymbol{A}(\boldsymbol{x}(t), t), \tag{2.13}$$

with initial condition $\boldsymbol{x}(t_0) = \boldsymbol{x}_0$. The corresponding propagator is

$$p(\boldsymbol{z}, t|\boldsymbol{x}_0, t_0) = \delta(\boldsymbol{z} - \boldsymbol{x}(t)), \tag{2.14}$$

with the initial condition

$$p(\boldsymbol{z}, t_0|\boldsymbol{x}_0, t_0) = \delta(\boldsymbol{z} - \boldsymbol{x}_0). \tag{2.15}$$

By calculating the time derivative of Eq. (2.14), one shows that it solves indeed the Chapman–Kolmogorov equation,

$$\begin{aligned}\frac{\partial}{\partial t}p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0) &= -\sum_i \left(\frac{\mathrm{d}}{\mathrm{d}t}x_i(t)\right)\frac{\partial}{\partial z_i}\delta(\boldsymbol{z}-\boldsymbol{x}(t)) \\ &= -\sum_i A_i(\boldsymbol{x}(t),t)\frac{\partial}{\partial z_i}\delta(\boldsymbol{z}-\boldsymbol{x}(t)) \\ &= -\sum_i \frac{\partial}{\partial z_i}\left[A_i(\boldsymbol{z},t)p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0)\right], \end{aligned} \tag{2.16}$$

where Eq. (2.13) is used in the second line. Equation (2.16) coincides with the Chapman–Kolmogorov equation (2.12) for vanishing diffusion matrix and transition rate.

2.2.2. Diffusive motion

The situation becomes more involved if there is, in addition to the drift vector $\boldsymbol{A}(\boldsymbol{z},t)$, a nonvanishing diffusion matrix $\mathsf{D}(\boldsymbol{z},t)$. Equation (2.12) then becomes a *Fokker–Planck equation* that describes diffusive behavior,

$$\frac{\partial}{\partial t}p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0) = -\sum_i \frac{\partial}{\partial z_i}\left[A_i(\boldsymbol{z},t)p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0)\right]+\frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i\partial z_j}\left[D_{ij}(\boldsymbol{z},t)p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0)\right]. \tag{2.17}$$

At first, consider the simplest one-dimensional case with constant drift A and diffusion constant D. By using the same initial condition as in Eq. (2.15), which characterizes a definite initial state, and by going into Fourier space, one obtains the solution

$$p(z,t_0+\Delta t|x_0,t_0) = \frac{1}{\sqrt{2\pi D\Delta t}}\exp\left(-\frac{(z-x_0-A\Delta t)^2}{2D\Delta t}\right). \tag{2.18}$$

Equation (2.18) is a Gaussian with mean value $x_0+A\Delta t$ and a variance $D\Delta t$ that grows linearly in time. An analogous calculation in d dimensions yields the Gaussian

$$\begin{aligned}p(\boldsymbol{z},t+\Delta t|\boldsymbol{x}_0,t_0) = &\frac{1}{(2\pi\Delta t)^{d/2}\sqrt{\det\mathsf{D}}} \\ &\times\exp\left[-\frac{1}{2\Delta t}\left(\boldsymbol{z}-\boldsymbol{x}_0-\boldsymbol{A}\Delta t\right)^{\mathrm{T}}\mathsf{D}^{-1}\left(\boldsymbol{z}-\boldsymbol{x}_0-\boldsymbol{A}\Delta t\right)\right]. \end{aligned} \tag{2.19}$$

For the general case of time-dependent and inhomogeneous drift vectors and diffusion matrices, Eq. (2.19) still captures approximately the short-time behavior of a solution with initial distribution (2.15) because the spatial and temporal dependences are negligible for δ-like distributions and short times [41].

Irregularity of trajectories The trajectories that build the ensemble described by $p(\boldsymbol{z}, t|\boldsymbol{x}_0, t_0)$ cannot be described by the deterministic ordinary differential equation (2.13) because, as we just saw, the solution broadens in the course of the evolution meaning an increase of the ignorance about the distribution with time. An indicator for this non-ordinary behavior is the irregularity of the trajectories that is depicted by investigating their continuousness and differentiability. For simplicity, I consider the one-dimensional case with propagator (2.18). For Markov processes, it holds that the trajectories are almost surely continuous [41] if for arbitrary $\varepsilon > 0$

$$\lim_{h\to 0} \frac{1}{h} \mathrm{Prob}\left(|x(t_0+h) - x_0| > \varepsilon\right) = 0. \tag{2.20}$$

By noting that $\mathrm{Prob}\left(|\Delta| > \varepsilon\right) = \mathrm{Prob}\left(\Delta > \varepsilon\right) + \mathrm{Prob}\left(-\Delta > \varepsilon\right)$, with $\Delta = x(t_0+h) - x_0$, one uses (2.18) to get

$$\begin{aligned} \mathrm{Prob}\left(\pm\Delta > \varepsilon\right) &= \int_{\varepsilon}^{\infty} p(x_0 \pm \Delta, t_0 + h|x_0, t_0)\mathrm{d}\Delta \\ &= \int_{\varepsilon}^{\infty} \frac{\exp\left(-\left(\Delta \mp Ah\right)^2/2Dh\right)}{\sqrt{2\pi Dh}}\mathrm{d}\Delta = \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{\varepsilon \mp Ah}{\sqrt{2Dh}}\right)\right], \end{aligned} \tag{2.21}$$

where $\mathrm{erf}\left(\cdot\right)$ is the Gaussian error function. If one inserts Eq. (2.21) into the left-hand side of Eq. (2.20) and uses l'Hôpital's rule one can confirm that the trajectories described by the Fokker–Planck equation (2.17) are continuous. On the other hand, by a similar calculation one shows that the trajectories are almost surely *not* differentiable, i.e. for arbitrary $\varepsilon > 0$

$$\lim_{h\to 0} \mathrm{Prob}\left(\frac{|x(t_0+h) - x_0|}{h} > \varepsilon\right) = 1. \tag{2.22}$$

To evaluate Eq. (2.22), one has to calculate the integral

$$\begin{aligned} \mathrm{Prob}\left(\pm\Delta > h\varepsilon\right) &= \int_{h\varepsilon}^{\infty} p(x_0 \pm \Delta, t_0 + h|x_0, t_0)\mathrm{d}\Delta \\ &= \int_{h\varepsilon}^{\infty} \frac{\exp\left(-\left(\Delta \mp Ah\right)^2/2Dh\right)}{\sqrt{2\pi Dh}}\mathrm{d}\Delta = \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{\left(\varepsilon \mp A\right)h}{\sqrt{2Dh}}\right)\right]. \end{aligned} \tag{2.23}$$

Taking the limit $h \to 0$ of Eq. (2.23) leads to Eq. (2.22), which implies that the difference quotient exceeds every bound with probability one in the limit $h \to 0$ and therefore the differential quotient does not exist.

2.2.3. Jump motion

The third process that is described by the differential Chapman-Kolmogorov equation (2.12) occurs when there is a nonvanishing transition rate $W(\boldsymbol{z}|\boldsymbol{x},t)$ alongside a vanishing drift vector and diffusion matrix. One obtains the *jump master equation*

$$\frac{\partial}{\partial t}p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0) = \int \mathrm{d}\boldsymbol{y}\left[W(\boldsymbol{z}|\boldsymbol{y},t)p(\boldsymbol{y},t|\boldsymbol{x}_0,t_0) - W(\boldsymbol{y}|\boldsymbol{z},t)p(\boldsymbol{z},t|\boldsymbol{x}_0,t_0)\right]. \tag{2.24}$$

Again, one possesses full knowledge of the initial state according to the initial condition (2.15). The propagator can then be approximated to first order in the timestep Δt,

$$p(\boldsymbol{z},t_0+\Delta t|\boldsymbol{x}_0,t_0) = \delta(\boldsymbol{z}-\boldsymbol{x}_0)\left(1-\int W(\boldsymbol{y}|\boldsymbol{x}_0,t_0)\mathrm{d}\boldsymbol{y}\Delta t\right) + W(\boldsymbol{z}|\boldsymbol{x}_0,t_0)\Delta t, \tag{2.25}$$

where the factor to the right of $\delta(\cdot)$ represents the probability to stay at the initial position $\boldsymbol{x}_0$, and $W(\boldsymbol{z}|\boldsymbol{x}_0,t_0)\Delta t$ is, upon normalization, the probability density that a jump to position $\boldsymbol{z}$ occurs.

Waiting-time distribution An important quantity for the characterization as well as for the simulation of these processes is the so-called *waiting-time distribution* [41]; that is the probability distribution $f(\tau|\boldsymbol{x},t)\mathrm{d}\tau$ for the time τ between two consecutive jumps, provided a jump occured at time t to the position $\boldsymbol{x}$. Its cumulative distribution function is calculated via integration,

$$F(\tau|\boldsymbol{x},t) = \int_0^\tau f(t'|\boldsymbol{x},t)\mathrm{d}t', \tag{2.26}$$

and it describes the probability for the next jump to occur in the interval $[t,t+\tau]$ when a jump occured at time t. With these two definitions it is straightforward to see that

$$\mathrm{d}F(\tau|\boldsymbol{x},t) = f(\tau|\boldsymbol{x},t)\mathrm{d}\tau = (1-F(\tau|\boldsymbol{x},t))\,\Gamma\left(\boldsymbol{x},t+\tau\right)\mathrm{d}\tau, \tag{2.27}$$

where the first factor on the right-hand side is the probability that no jump occurs in the interval $[t,t+\tau]$ and the second one is the total jump rate

$$\Gamma(\boldsymbol{x},t+\tau) = \int W(\boldsymbol{y}|\boldsymbol{x},t+\tau)\mathrm{d}\boldsymbol{y}, \tag{2.28}$$

at position $\boldsymbol{x}$ and time $t+\tau$. The solution of Eq. (2.27) reads

$$F(\tau|\boldsymbol{x},t) = 1-\exp\left(-\int_0^\tau \Gamma\left(\boldsymbol{x},t+t'\right)\mathrm{d}t'\right), \tag{2.29}$$

and upon derivation with respect to τ one derives the waiting time distribution

$$f(\tau|\boldsymbol{x},t) = \Gamma\left(\boldsymbol{x},t+\tau\right)\exp\left(-\int_0^\tau \Gamma\left(\boldsymbol{x},t+t'\right)\mathrm{d}t'\right). \tag{2.30}$$

In case of a constant jump rate $\Gamma(t) \equiv \Gamma$, Eq. (2.30) simplifies to the exponential $f(\tau) = \Gamma \exp(-\Gamma\tau)$; the process is then called *homogeneous*. In general, when $\Gamma(t)$ has a non-trivial time-dependence, the process is called *inhomogeneous*.

We thus see that the motion described by the jump master equation (2.24) consists of time intervals where nothing happens and jumps at discrete times, with exponentially distributed jump times in the homogeneous case and jump times according to Eq. (2.30) in the inhomogeneous case. The incorporation of a drift term is straightforward and leads to trajectories that are piecewise deterministic as described by the ordinary differential equation (2.13) interrupted by jumps. The stochastic trajectories that lead to this behavior are discussed in Section 2.5.

2.3. Continuous processes

I now discuss in more detail the properties of the trajectories exhibited by a diffusive motion. It leads to the definition of a stochastic differential equation that describes their temporal evolution.

2.3.1. Wiener process

The one-dimensional Wiener process $W(t)$ is defined by the trajectories of the particular one-dimensional version of the diffusion equation (2.17) without drift, i.e. $A = 0$, with diffusion constant $D = 1$ and initial condition $p(w, t_0|w_0, t_0) = \delta(w - w_0)$. From Eqs. (2.17) and (2.18) one obtains the differential equation

$$\frac{\partial}{\partial t} p(w, t|w_0, t_0) = \frac{1}{2} \frac{\partial^2}{\partial w^2} p(w, t|w_0, t_0), \tag{2.31}$$

with its solution

$$p(w, t|w_0, t_0) = \frac{1}{\sqrt{2\pi(t - t_0)}} \exp\left(-\frac{(w - w_0)^2}{2(t - t_0)}\right). \tag{2.32}$$

This means that the Wiener process is a stochastic process with Gaussian distribution (2.32).

Independence of Wiener increments It is easily shown from the above definition of the Wiener process that the increments

$$\Delta W_i = W(t_i) - W(t_{i-1}) \tag{2.33}$$

are independent stochastic variables as introduced by Eq. (2.7).[1] One considers the joint probability density (2.5)

$$p(w_n, t_n; \ldots; w_0, t_0) = \prod_{i=1}^{n} p(w_i, t_i|w_{i-1}, t_{i-1}) p(w_0, t_0), \tag{2.34}$$

[1] Here and in the following, it is assumed that the time intervals associated with two Wiener increments are non-overlapping.

and inserts the propagator (2.32) to get

$$p(w_n,t_n;\ldots;w_1,t_1;w_0,t_0)=\prod_{i=1}^{n}\frac{1}{\sqrt{2\pi(t_i-t_{i-1})}}\exp\left(-\frac{(w_i-w_{i-1})^2}{2(t_i-t_{i-1})}\right)p(w_0,t_0). \tag{2.35}$$

The joint probability density for the increments ΔW_i then reads

$$\begin{aligned}p(\Delta w_n;\ldots;\Delta w_1;w_0)&=p(w_n,t_n;\ldots;w_0,t_0)\\&=\prod_{i=1}^{n}\frac{1}{\sqrt{2\pi\Delta t_i}}\exp\left(-\frac{(\Delta w_i)^2}{2\Delta t_i}\right)p(w_0,t_0)\\&=\prod_{i=1}^{n}p(\Delta w_i)p(w_0,t_0),\end{aligned} \tag{2.36}$$

with $\Delta t_i = t_i - t_{i-1}$. Comparison with Eq. (2.7) confirms that the increments are mutually stochastically independent and independent of the initial value w_0.

Ensemble averages The ensemble averages are calculated straightforwardly using Eq. (2.9) with the propagator (2.32) of the Wiener process. For the first and second moments, one gets

$$\begin{aligned}\mathrm{E}\left[W(t)\right]&=w_0,\\\mathrm{E}\left[W(t)^2\right]&=w_0^2+t-t_0,\\\mathrm{E}\left[W(s)W(t)\right]&=w_0^2+\min(s-t_0,t-t_0).\end{aligned} \tag{2.37}$$

To see the third equation, one assumes, without loss of generality, that $s>t$ and rewrites $W(s)W(t)=\left(W(s)-W(t)\right)W(t)+W(t)^2$. Then one can use that $W(s)-W(t)$ is stochastically independent of $W(t)$, which, according to Eq. (2.7), allows one to factorize and evaluate the first summand,

$$\mathrm{E}\left[\left(W(s)-W(t)\right)W(t)\right]=\mathrm{E}\left[W(s)-W(t)\right]\mathrm{E}\left[W(t)\right]=0. \tag{2.38}$$

The calculation of the second moment at different times is therefore reduced to the calculation of the second moment at the same time; treating the case $t>s$ analogously confirms the above statement.

Using the averages (2.37), one directly calculates the first and second moments of the increments,

$$\begin{aligned}\mathrm{E}\left[\Delta W_i\right]&=0,\\\mathrm{E}\left[\left(\Delta W_i\right)^2\right]&=\Delta t_i,\\\mathrm{E}\left[\Delta W_i\Delta W_j\right]&=0,\end{aligned} \tag{2.39}$$

where $i\neq j$ and the third equation follows directly from the stochastic independence of the Wiener increments.

2.3.2. Stochastic integral

Now, I want to introduce an integral over the Wiener process. However, since $W(t)$ is stochastic, one has to pay special attention to unambigiously and consistently define such an object, see e.g. Ref. [45].

To start with the simplest case of an integral, consider the *Riemann integral* of an arbitrary function $G(t)$ over the interval $[t_0, t]$. By dividing the integration interval into subintervals $t_0 \leq t_1 \leq \cdots \leq t_{n-1} \leq t_n = t$, it is defined as the limit

$$\int_{t_0}^{t} G(t')\mathrm{d}t' := \lim_{n\to\infty} S_n \tag{2.40}$$

of the partial sum

$$S_n = \sum_{i=1}^{n} G(\tau_i)\,(t_i - t_{i-1})\,, \tag{2.41}$$

with $\tau_i \in [t_{i-1}, t_i]$. As is known, this definition is independent of the choice of the intermediate points τ_i; for example, set $\tau_i = t_i$. One may consider this integration procedure as integrating with respect to a straight line.

A generalization of the Riemann integral arises if one integrates the function $G(t)$ with respect to another function, say $H(t)$. The ensuing *Riemann–Stieltjes integral* is defined as the limit $n \to \infty$ of the partial sum

$$S_n = \sum_{i=1}^{n} G(\tau_i)\,[H(t_i) - H(t_{i-1})]\,. \tag{2.42}$$

If $H(t)$ is differentiable one can transform this integral into a Riemann integral by substitution:

$$\int_{t_0}^{t} G(t')\mathrm{d}H(t') = \int_{t_0}^{t} G(t')\frac{\mathrm{d}H(t')}{\mathrm{d}t'}\mathrm{d}t'. \tag{2.43}$$

The situation changes when an integration along the Wiener process $W(t)$ is done, since its paths are stochastic and non-differentiable. Therefore, the limit of the sum

$$S_n = \sum_{i=1}^{n} G(\tau_i)\,[W(t_i) - W(t_{i-1})] \tag{2.44}$$

has to be defined in an ensemble sense. In particular, one takes the *mean-square limit*,

$$\underset{n\to\infty}{\text{ms-lim}}\, S_n = S \quad \Leftrightarrow \quad \lim_{n\to\infty} \mathrm{E}\left[(S_n - S)^2\right] = 0. \tag{2.45}$$

where, in contrast to the preceeding two integral definitions, the value S of the integral does depend on the choice of the intermediate points τ_i, at which the integrand $G(\tau_i)$

is evaluated. Choosing the left border of each subinterval, $\tau_i = t_{i-1}$ for all i, leads to the *stochastic Ito integral* [41, 45]

$$\int_{t_0}^{t} G(t')\mathrm{d}W(t') := \underset{n\to\infty}{\text{ms-lim}} \sum_{i=1}^{n} G(t_{i-1})\Delta W_i. \tag{2.46}$$

Stochastic independence of the integrand The integrand $G(t)$, though arbitrary, is assumed to be *non-anticipating*, which means that $G(t')$ may depend, apart from the time t', on the Wiener process $W(t')$ for times $t' < t$ only. This is in accordance with causality, requiring that the function should not depend on events at future times. For the Ito choice of the intermediate points, $\tau_i = t_{i-1}$, one deduces immediately that every non-anticipating integrand is stochastically independent of the integrator $\mathrm{d}W(t')$, which is convenient for evaluating the stochastic integral.

The Ito rules of stochastic calculus There are basically two rules, which turn calculations of the Ito integral into a straightforward subject. They state, loosely speaking, that the differential $\mathrm{d}W(t)$ can be handled like an infinitesimal of order $\mathrm{d}t^{1/2}$ and that in calculations terms up to first order in $\mathrm{d}t$ only are kept. Since the differential $\mathrm{d}W(t)$ is only defined via the Ito integral (2.46), the Ito rules must be understood to apply below this integral for arbitrary non-anticipating functions $G(t)$. One can confirm by direct calculation, see e.g. Ref. [41]

$$\begin{aligned}
\int_{t_0}^{t} G(t') \left[\mathrm{d}W(t')\right]^2 &= \int_{t_0}^{t} G(t')\mathrm{d}t', \\
\int_{t_0}^{t} G(t')\mathrm{d}W(t')\mathrm{d}t &= 0, \\
\int_{t_0}^{t} G(t') \left[\mathrm{d}W(t')\right]^{2+N} &= 0,
\end{aligned} \tag{2.47}$$

with $N \geq 1$. The shorthand notation for the differentials gives the *Ito rules*

$$\begin{aligned}
\left[\mathrm{d}W(t)\right]^2 &= \mathrm{d}t, \\
\mathrm{d}W(t)\mathrm{d}t &= 0, \\
\left[\mathrm{d}W(t)\right]^{2+N} &= 0.
\end{aligned} \tag{2.48}$$

One infers that $\mathrm{d}W(t)$ can be treated as a differential of order $\mathrm{d}t^{1/2}$. In addition, from Eqs. (2.39) one deduces for the ensemble average of the infinitesimal Wiener increment

$$\mathrm{E}\left[\mathrm{d}W(t)\right] = 0. \tag{2.49}$$

Multivariate Wiener processes The above discussion can be easily generalized to the Wiener process in d dimensions

$$\boldsymbol{W}(t) = [W_1(t), \ldots, W_d(t)], \tag{2.50}$$

where the $W_i(t)$ are independent one-dimensional Wiener processes. Due to the stochastic independence of the corresponding one-dimensional increments one gets the *multi-dimensional Ito rules*

$$\begin{aligned} \mathrm{d}W_i(t)\mathrm{d}W_j(t) &= \delta_{ij}\mathrm{d}t, \\ \mathrm{d}W_i(t)\mathrm{d}t &= 0, \\ \mathrm{d}W_i(t)\mathrm{d}W_j(t)\ldots\mathrm{d}W_k(t) &= 0. \end{aligned} \tag{2.51}$$

Stratonovich integral As stated above, the stochastic integral defined in Eqs. (2.44) and (2.45) depends on the choice of the intermediate points τ_i at which the integrand $G(\tau_i)$ is evaluated; moreover, the Ito integral corresponds to $\tau_i = t_{i-1}$. The second prominent stochastic integral, the *Stratonovich integral*, arises by taking as integrand the arithmetic mean $\left(G(t_{i-1}) + G(t_i)\right)/2$. The rules of calculation with this integral coincide with the rules of ordinary integral calculus. Since the Stratonovich integral is not used in this thesis, I omit the discussion of its properties here.

2.3.3. Stochastic differential equations

It is now possible to give a meaning to a differential equation involving the d-dimensional Wiener increment $\mathrm{d}\boldsymbol{W}(t)$ by use of the Ito integral (2.46). In particular, for the differential $\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{x}(t + \mathrm{d}t) - \boldsymbol{x}(t)$ one writes down the *stochastic differential equation* (SDE)

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{A}\left(\boldsymbol{x}(t), t\right)\mathrm{d}t + \mathsf{B}\left(\boldsymbol{x}(t), t\right)\mathrm{d}\boldsymbol{W}(t), \tag{2.52}$$

with the drift vector $\boldsymbol{A}(\boldsymbol{x}(t), t)$ and the matrix $\mathsf{B}\left(\boldsymbol{x}(t), t\right)$ describing the diffusive properties. The SDE attains a meaning by defining as its solution the stochastic trajectory

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_0) + \int_{t_0}^{t} \boldsymbol{A}\left(\boldsymbol{x}(t'), t'\right)\mathrm{d}t' + \int_{t_0}^{t} \mathsf{B}\left(\boldsymbol{x}(t'), t'\right)\mathrm{d}\boldsymbol{W}(t'). \tag{2.53}$$

The Ito lemma Together with the Ito rules from Eqs. (2.51), one can go over from the SDE (2.52) to a SDE for the function $f(\boldsymbol{x}(t), t)$ of the trajectory, which is known as the *Ito lemma*. For its derivation, one calculates the differential $\mathrm{d}f(\boldsymbol{x}(t), t) = f\left(\boldsymbol{x}(t) + \mathrm{d}\boldsymbol{x}(t), t + \mathrm{d}t\right) - f(\boldsymbol{x}(t), t)$ by performing the Taylor expansion,

$$\mathrm{d}f(\boldsymbol{x}(t), t) = \frac{\partial f(\boldsymbol{x}(t), t)}{\partial t}\mathrm{d}t + \sum_{i=1}^{d} \frac{\partial f(\boldsymbol{x}(t), t)}{\partial x_i}\mathrm{d}x_i(t) + \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2 f(\boldsymbol{x}(t), t)}{\partial x_i \partial x_j}\mathrm{d}x_i(t)\mathrm{d}x_j(t). \tag{2.54}$$

Plugging in the SDE (2.52) and using the Ito rules (2.51), one obtains up to first order in $\mathrm{d}t$,

$$\mathrm{d}f(\boldsymbol{x},t) = \left(\frac{\partial f(\boldsymbol{x},t)}{\partial t} + \sum_{i=1}^{d} \frac{\partial f(\boldsymbol{x},t)}{\partial x_i} A_i(\boldsymbol{x},t) + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 f(\boldsymbol{x},t)}{\partial x_i \partial x_j} \left(\mathsf{B}\mathsf{B}^{\mathrm{T}}\right)_{ij} (\boldsymbol{x},t) \right) \mathrm{d}t + \sum_{i=1}^{d} \frac{\partial f(\boldsymbol{x},t)}{\partial x_i} \left(\mathsf{B}\mathrm{d}\boldsymbol{W}\right)_i (\boldsymbol{x},t) \,. \quad (2.55)$$

Here and in the following, I omit the time argument of the trajectory and of the Wiener increment for a better readability, i.e. $\boldsymbol{x} \equiv \boldsymbol{x}(t)$ and $\mathrm{d}\boldsymbol{W} \equiv \mathrm{d}\boldsymbol{W}(t)$. Notice that higher than second order terms in the expansion of $\mathrm{d}f(\boldsymbol{x},t)$ lead to differentials at least of order $(\mathrm{d}t)^{3/2}$, which do not contribute to the SDE (2.55), and are therefore neglected.

As a simple example, consider the function $f(\boldsymbol{x},t) = x_k^2$. The differential equation for $\mathrm{d}\left(x_k^2\right)$ is readily derived by evaluation of Eqs. (2.54) and (2.55):

$$\begin{aligned} \mathrm{d}\left(x_k^2\right) &= 2x_k \mathrm{d}x_k + (\mathrm{d}x_k)^2 \\ &= \left(2x_k A_k(\boldsymbol{x},t) + \sum_{j=1}^{d} B_{kj}(\boldsymbol{x},t)^2 \right) \mathrm{d}t + 2x_k \sum_{j=1}^{d} B_{kj}(\boldsymbol{x},t) \mathrm{d}W_j . \end{aligned} \quad (2.56)$$

With this SDE for $\mathrm{d}\left(x_k^2\right)$, it is straightforward to write down a SDE for the associated variance of the trajectory, $\mathrm{Var}\left[x_k\right] = \mathrm{E}\left[x_k^2\right] - \mathrm{E}\left[x_k\right]^2$,

$$\mathrm{d}\mathrm{Var}\left[x_k\right] = \mathrm{E}\left[\mathrm{d}\left(x_k^2\right)\right] - 2\mathrm{E}\left[x_k\right]\mathrm{E}\left[\mathrm{d}x_k\right] . \quad (2.57)$$

Connection to the Fokker–Planck equation From the trajectories defined by the SDE (2.52) one can arrive at an equation of motion for the accompanied probability density, which turns out to be a Fokker–Planck equation of type (2.17). For simplicity, I restrict the calculation to the one-dimensional case, where the SDE (2.52) simplifies to the form

$$\mathrm{d}x = A(x,t)\,\mathrm{d}t + B(x,t)\,\mathrm{d}W. \quad (2.58)$$

At first, one considers an arbitrary function $f(x)$ that does not explicitly depend on time and calculates the time derivative of its ensemble average. It reads

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}\left[f(x)\right] &\equiv \frac{1}{\mathrm{d}t}\mathrm{E}\left[\mathrm{d}f(x)\right] \\ &= \frac{1}{\mathrm{d}t}\mathrm{E}\left[\left(A(x,t)\frac{\partial f(x)}{\partial x} + \frac{1}{2}B(x,t)^2\frac{\partial^2 f(x)}{\partial x^2} \right)\mathrm{d}t + B(x,t)\frac{\partial f(x)}{\partial x}\mathrm{d}W\right], \end{aligned} \quad (2.59)$$

where the SDE (2.58) and the one-dimensional version of the Ito lemma (2.55) is used. Notice that the term that includes the Wiener increment vanishes in the ensemble

average, see Eq. (2.49). In a second step, one represents the ensemble average $\mathrm{E}[\cdot]$ by an integral over the probability density $p(x,t|x_0,t_0)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}[f(x)] = \frac{\mathrm{d}}{\mathrm{d}t}\int f(y)p(y,t|x_0,t_0)\mathrm{d}y = \int f(y)\frac{\partial}{\partial t}p(y,t|x_0,t_0)\mathrm{d}y. \tag{2.60}$$

The ensemble averages on both sides of Eq. (2.59) are now rewritten with the help of Eq. (2.60) and the right-hand side is integrated by parts. One gets

$$\int \mathrm{d}y\, f(y)\frac{\partial}{\partial t}p(y,t|x_0,t_0) = \int \mathrm{d}y\, f(y)\Big\{ -\frac{\partial}{\partial y}\left[A(y,t)p(y,t|x_0,t_0)\right] + \frac{1}{2}\frac{\partial^2}{\partial y^2}\left[B(y,t)^2 p(y,t|x_0,t_0)\right]\Big\}. \tag{2.61}$$

Because Eq. (2.61) holds for every $f(x)$, it is already true without the integral, which finally leads to the Fokker–Planck equation

$$\frac{\partial}{\partial t}p(x,t|x_0,t_0) = -\frac{\partial}{\partial x}\left[A(x,t)p(x,t|x_0,t_0)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[B(x,t)^2 p(x,t|x_0,t_0)\right]. \tag{2.62}$$

Multi-dimensional case In d dimensions, one can find in the same way that the SDE (2.52) is associated to the Fokker–Planck equation (2.17), where the diffusion matrix in Eq. (2.17) is defined by $\mathsf{D}(\boldsymbol{x}(t),t) = \mathsf{B}\mathsf{B}^{\mathrm{T}}(\boldsymbol{x}(t),t)$.

2.4. Example: diffusion in phase space

As a specific stochastic model, let us consider the SDE

$$\begin{pmatrix} \mathrm{d}x(t) \\ \mathrm{d}p(t) \end{pmatrix} = \begin{pmatrix} p(t) \\ -p(t) \end{pmatrix}\mathrm{d}t + \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}\begin{pmatrix} \mathrm{d}W_1(t) \\ \mathrm{d}W_2(t) \end{pmatrix}, \tag{2.63}$$

which is a special case of the Ornstein–Uhlenbeck process, see Ref. [41]. Let $x(t)$ and $p(t)$ be the dimensionless position and momentum variable; then Eq. (2.63) describes a diffusion process in phase space with constant real coefficients B_{ij}. It will be convenient to take as time, length, and momentum units

$$\mathrm{T} = \frac{1}{2\gamma}, \quad \mathrm{L} = \frac{1}{2\gamma}\sqrt{\frac{k_{\mathrm{B}}T}{m}}, \quad \mathrm{P} = \sqrt{mk_{\mathrm{B}}T}, \tag{2.64}$$

with friction coefficient γ, temperature T and particle mass m. The time dependence of x, p and of the Wiener increments $\mathrm{d}W_1$ and $\mathrm{d}W_2$ is omitted in what follows.

In the next section, the ensemble properties of the process (2.63) are examined by deriving equations of motion for various ensemble averages and solving them.

2.4.1. Equations of motion for ensemble averages

First moments Taking the ensemble average of Eq. (2.63) yields

$$\begin{aligned} \mathrm{E}[\mathrm{d}x] &= \mathrm{E}[p]\mathrm{d}t, \\ \mathrm{E}[\mathrm{d}p] &= -\mathrm{E}[p]\mathrm{d}t, \end{aligned} \tag{2.65}$$

with solutions

$$\begin{aligned} \mathrm{E}[x] &= x_0 + p_0\left(1 - \mathrm{e}^{-t}\right), \\ \mathrm{E}[p] &= p_0\mathrm{e}^{-t}. \end{aligned} \tag{2.66}$$

Here, the initial conditions $x(0) = x_0$ and $p(0) = p_0$ are used.

Variances The variances of the position and momentum, $\mathrm{Var}[x]$ and $\mathrm{Var}[p]$, as well as the covariance $\mathrm{Cov}[x, p]$ are defined by

$$\begin{aligned} \mathrm{Var}[x] &= \mathrm{E}[x^2] - \mathrm{E}[x]^2, \\ \mathrm{Var}[p] &= \mathrm{E}[p^2] - \mathrm{E}[p]^2, \\ \mathrm{Cov}[x, p] &= \mathrm{E}[xp] - \mathrm{E}[x]\mathrm{E}[p]. \end{aligned} \tag{2.67}$$

As demonstrated in Section 2.3.3, for the derivation of their equations of motion, one first calculates the equations of motion for the involved second moments. They read

$$\begin{aligned} \mathrm{E}\left[\mathrm{d}\left(x^2\right)\right] &= \mathrm{E}[2x\mathrm{d}x] + \mathrm{E}[(\mathrm{d}x)^2] = \left(2\mathrm{E}\left[xp\right] + D_x\right)\mathrm{d}t, \\ \mathrm{E}\left[\mathrm{d}\left(p^2\right)\right] &= \mathrm{E}[2p\mathrm{d}p] + \mathrm{E}[(\mathrm{d}p)^2] = \left(-2\mathrm{E}\left[p^2\right] + D_p\right)\mathrm{d}t, \\ \mathrm{E}\left[\mathrm{d}\left(xp\right)\right] &= \mathrm{E}[x\mathrm{d}p + p\mathrm{d}x] + \mathrm{E}[\mathrm{d}x\mathrm{d}p] = \left(-\mathrm{E}\left[xp\right] + \mathrm{E}[p^2] + D_{xp}\right)\mathrm{d}t, \end{aligned} \tag{2.68}$$

where the SDE (2.63) is used and one makes use of the definition of the diffusion constants D_x and D_p and the covariance diffusion D_{xp},

$$\begin{aligned} D_x &= B_{11}^2 + B_{12}^2, \\ D_p &= B_{21}^2 + B_{22}^2, \\ D_{xp} &= B_{11}B_{21} + B_{12}B_{22}. \end{aligned} \tag{2.69}$$

The ensuing equations of motion read

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[x] &= 2\mathrm{Cov}[x, p] + D_x, \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[p] &= -2\mathrm{Var}[p] + D_p, \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cov}[x, p] &= -\mathrm{Cov}[x, p] + \mathrm{Var}[p] + D_{xp}, \end{aligned} \tag{2.70}$$

which are straightforwardly solved by successively calculating $\mathrm{Var}\left[p\right]$, $\mathrm{Cov}\left[x, p\right]$, and $\mathrm{Var}\left[x\right]$. Denoting the initial values as $\mathrm{Var}\left[x\right]_0$, $\mathrm{Var}\left[p\right]_0$, and $\mathrm{Cov}\left[x, p\right]_0$, one gets

$$\begin{aligned}
\mathrm{Var}[x] &= \mathrm{Var}\,[x]_0 + (D_x + D_p + 2D_{xp})\,t + \left(\mathrm{Var}\,[p]_0 - \frac{1}{2}D_p\right)\left(1-\mathrm{e}^{-t}\right)^2 \\
&\quad + \left(2\mathrm{Cov}\,[x,p]_0 - D_p - 2D_{xp}\right)\left(1-\mathrm{e}^{-t}\right), \\
\mathrm{Var}[p] &= \mathrm{Var}\,[p]_0\,\mathrm{e}^{-2t} + \frac{1}{2}D_p\left(1-\mathrm{e}^{-2t}\right), \\
\mathrm{Cov}[x,p] &= \mathrm{Cov}\,[x,p]_0\,\mathrm{e}^{-t} + \left(\mathrm{Var}\,[p]_0\,\mathrm{e}^{-t} + D_{xp}\right)\left(1-\mathrm{e}^{-t}\right) + \frac{1}{2}D_p\left(1-\mathrm{e}^{-t}\right)^2.
\end{aligned} \tag{2.71}$$

2.4.2. Phase space description

The associated Fokker–Planck equation to the SDE (2.63), is readily derived with the help of the discussion in Section 2.3.3. For the probability density $f(x,p,t)$ one gets

$$\begin{aligned}
\frac{\partial}{\partial t}f\,(x,p,t) &= -p\frac{\partial}{\partial x}f\,(x,p,t) + \frac{\partial}{\partial p}\left[pf\,(x,p,t)\right] \\
&\quad + \frac{D_x}{2}\frac{\partial^2}{\partial x^2}f\,(x,p,t) + \frac{D_p}{2}\frac{\partial^2}{\partial p^2}f\,(x,p,t) + D_{xp}\frac{\partial^2}{\partial x\partial p}f\,(x,p,t),
\end{aligned} \tag{2.72}$$

with the initial condition $f(x,p,t_0) = f\,(x_0,p_0)$.

2.4.3. Classical Brownian motion

A simplified case of the above phase space diffusion arises if one sets $B_{11} = B_{12} = 0$ in Eq. (2.63). It then follows from the definition of the diffusion constants, Eqs. (2.69), that D_p is nonvanishing, whereas $D_x = D_{xp} = 0$. Equation (2.63) turns into a deterministic equation for the position, $\mathrm{d}x = p\mathrm{d}t$, and into a SDE for the momentum,

$$\mathrm{d}p = -p\mathrm{d}t + \sqrt{D_p}\mathrm{d}W, \tag{2.73}$$

with the single Wiener increment $\mathrm{d}W$. Here, it is used that $\sqrt{D_p}\mathrm{d}W = B_{21}\mathrm{d}W_1 + B_{22}\mathrm{d}W_2$, which is seen by comparing the ensemble averages $\mathrm{E}\left[(\cdot)^n\right]$ for $n \geq 1$ of both sides of the equation. The particular case $D_p = 2$ is called *classical Brownian motion* (CBM) [42, 46].

Variances The equations of motion for the variances (2.71) simplify a lot in the case of CBM. For a definite initial state, i.e. $\mathrm{Var}\,[x]_0 = \mathrm{Var}\,[p]_0 = \mathrm{Cov}\,[x,p]_0 = 0$, one gets

$$\begin{aligned}
\mathrm{Var}[x] &= 2t - \left(1-\mathrm{e}^{-t}\right)^2 - 2\left(1-\mathrm{e}^{-t}\right), \\
\mathrm{Var}[p] &= 1-\mathrm{e}^{-2t}, \\
\mathrm{Cov}[x,p] &= \left(1-\mathrm{e}^{-t}\right)^2.
\end{aligned} \tag{2.74}$$

For comparison with textbook solutions of Brownian motion, e.g. Ref. [46], one usually calculates the mean-square displacement of the position instead of its variance,

$$\begin{aligned} \mathrm{E}\left[(x-x_0)^2\right] &= \mathrm{Var}[x] + (\mathrm{E}[x]-x_0)^2 \\ &= 2t + \left(p_0^2-1\right)\left(1-\mathrm{e}^{-t}\right)^2 - 2\left(1-\mathrm{e}^{-t}\right). \end{aligned} \tag{2.75}$$

For large times both the position variance shown in Eqs. (2.74) and the mean-square displacement grow linearly with time, this is the main characteristic of classical Brownian motion.

The time dependence of the position variance of the general phase space diffusion, as shown in Eqs. (2.71), also has a term directly proportional to time, albeit with a different prefactor, which is formed by a sum of the different diffusion constants.

Phase space description The Fokker–Planck equation of CBM is readily obtained from Eq. (2.72) and reads

$$\frac{\partial}{\partial t} f(x,p,t) = -p\frac{\partial}{\partial x} f(x,p,t) + \frac{\partial}{\partial p}\left(p f(x,p,t)\right) + \frac{\partial^2}{\partial p^2} f(x,p,t), \tag{2.76}$$

with initial condition $f(x,p,t_0) = f(x_0,p_0)$.

2.5. Piecewise deterministic processes

It is the purpose of this section to examine the trajectories leading to the jump motion of the differential Chapman–Kolmogorov equation (2.12). As opposed to the continuous stochastic processes with non-differentiable trajectories, one encounters piecewise deterministic trajectories which are interrupted by jumps of finite size. For introductions see e.g. Refs. [42, 43]

2.5.1. Poisson process

The Poisson process $N(t)$ counts the number of discrete, independent stochastic events, which occur with rate $\gamma(t)$. In case of an event, denoted as a jump, $N(t)$ increases by one. One may consider, for example, the arrival of electrons at the anode in a vacuum tube. The quantitiy of interest is the conditional probability density $p(n,t|n_0,t_0)$ describing the case that n events have occured up to time t provided one started with n_0 events at t_0. In analogy to the jump master equation (2.24), which is defined in continuous space, one can write down a master equation for the time evolution of the Poisson process. Two terms contribute to the temporal change of the probability density $p(n,t|n_0,t_0)$: The first one takes account for an increase proportional to $p(n-1,t|n_0,t_0)$ due to the jump $n-1 \to n$. The second term, which describes a decrease proportional to $p(n,t|n_0,t_0)$, results from the jump $n \to n+1$. Both jumps occur with a rate $\gamma(t)$ and lead to the master equation

$$\frac{\partial}{\partial t} p(n,t|n_0,t_0) = \gamma(t)\left[p(n-1,t|n_0,t_0) - p(n,t|n_0,t_0)\right], \tag{2.77}$$

where $n > n_0$.

As one easily verifies, Eq. (2.77) is solved by the propagator

$$p(n,t|n_0,t_0) = \mathrm{e}^{-\mu(t,t_0)} \frac{\mu\,(t,t_0)^{n-n_0}}{(n-n_0)!}, \tag{2.78}$$

with the integrated jump probability

$$\mu(t,t_0) = \int_{t_0}^{t} \gamma(t')\mathrm{d}t'. \tag{2.79}$$

Waiting-time distribution The waiting time distribution of the Poisson process, i.e. the distribution of the times between two jumps, is calculated similarly to that of the jump master equation (2.24). Namely, one multiplies the probability that no jump occurs in the interval $[t, t+\tau]$ and the jump rate at time $t+\tau$,

$$f(\tau|n,t) = \mathrm{e}^{-\mu(t+\tau,t)}\gamma(t+\tau), \tag{2.80}$$

where the first factor equals $p(n,t+\tau|n,t)$ and is deduced from the propagator (2.78). If the process is homogeneous, i.e. $\gamma(t) \equiv \gamma$, one obtains the exponential distribution $f(\tau) = \gamma \exp(-\gamma\tau)$.

Independence of Poisson increments The Poisson increments

$$\Delta N_i = N(t_i) - N(t_{i-1}), \tag{2.81}$$

with non-overlapping time increments $\Delta t_i = t_i - t_{i-1}$ are independent stochastic variables. To prove this, one calculates the joint probability (2.5) by using the propagator (2.78),

$$p(n_n,t_n;\ldots;n_1,t_1;n_0,t_0) = \prod_{i=1}^{n} \mathrm{e}^{-\mu(t_i,t_{i-1})} \frac{\mu\,(t_i,t_{i-1})^{n_i-n_{i-1}}}{(n_i-n_{i-1})!} p(n_0,t_0). \tag{2.82}$$

A reordering leads to the joint probability density for the increments $\Delta n_i = n_i - n_{i-1}$:

$$p(\Delta n_n,\Delta t_n;\ldots;\Delta n_1,\Delta t_1;n_0,t_0) = \prod_{i=1}^{n} p(\Delta n_i,\Delta t_i,t_{i-1}) p(n_0,t_0). \tag{2.83}$$

Thus, the Poisson increments are mutually independent and independent of the initial state $N(t_0)$.

Ensemble averages Similar to the Wiener process, the ensemble averages of the Poisson process are calculated with the help of the propagator (2.78). Note that the averaging involves a sum and not an integral as in Eq. (2.9), due to the discreteness of the Poisson process. For an arbitrary function $f(N(t))$ the ensemble average reads

$$\mathrm{E}\left[f\left(N(t)\right)\right] = \sum_{n=n_0}^{\infty} f(n) p(n,t|n_0,t_0). \tag{2.84}$$

For the first and second moments, this readily gives

$$\begin{aligned} \mathrm{E}\left[N(t)\right] &= n_0 + \mu(t,t_0), \\ \mathrm{E}\left[N(t)^2\right] &= \left[n_0 + \mu(t,t_0)\right]^2 + \mu(t,t_0), \\ \mathrm{E}\left[N(s)N(t)\right] &= n_0^2 + n_0\left[\mu(s,t_0) + \mu(t,t_0)\right] \\ &\quad + \mu\left(s,t_0\right)\mu(t,t_0) + \mu\left(\min\left(s,t\right),t_0\right). \end{aligned} \tag{2.85}$$

The third equation is derived by using the stochastic independence of the Poisson increments, analogous to the derivation of the corresponding equation for the Wiener process, as shown in Eqs. (2.37). Accordingly, the first and second moments of the Poisson increments are

$$\begin{aligned} \mathrm{E}\left[\Delta N_i\right] &= \mu(t_i,t_{i-1}), \\ \mathrm{E}\left[\left(\Delta N_i\right)^2\right] &= \mu(t_i,t_{i-1})^2 + \mu(t_i,t_{i-1}), \\ \mathrm{E}\left[\Delta N_i \Delta N_j\right] &= \mu(t_i,t_{i-1})\mu(t_j,t_{j-1}). \end{aligned} \tag{2.86}$$

Poisson increment rules For infinitesimal time increments $\mathrm{d}t$ one introduces the Poisson increments

$$\mathrm{d}N(t) = N(t) - N(t-\mathrm{d}t). \tag{2.87}$$

In spite of the suggestive notation, this increment is by no means infinitesimal, since the Poisson process counts whole events. In fact, the increment is zero if no jump occurs in the interval $[t, t+\mathrm{d}t]$ and it equals one if a jump occurs. The probability that more than one jump occurs is negligible. This already leads to the *Poisson rule*

$$\left[\mathrm{d}N(t)\right]^2 = \mathrm{d}N(t). \tag{2.88}$$

An insight, which one gets either from Eq. (2.88) or directly from the ensemble averages (2.86), is

$$\mathrm{E}\left[\mathrm{d}N(t)\right] = \mathrm{E}\left[\left[\mathrm{d}N(t)\right]^2\right] = \gamma(t)\mathrm{d}t, \tag{2.89}$$

where, according to Eq. (2.79), $\mu(t+\mathrm{d}t,t) \approx \gamma(t)\mathrm{d}t$ is used and only terms up to first order in $\mathrm{d}t$ are considered. This is in contrast to the Wiener process, where only the second moment of the increments is proportional to $\mathrm{d}t$. As one easily infers, all moments of the Poisson increments have a rate according to Eq. (2.89).

Multivariate case For several independent Poisson processes $\mathrm{d}N_k(t)$, there still occurs at most one jump in the infinitesimal time interval $\mathrm{d}t$, which leads to the *multivariate Poisson rule*

$$\mathrm{d}N_k(t)\mathrm{d}N_l(t) = \delta_{kl}\mathrm{d}N_k(t). \tag{2.90}$$

If the family of jumps is continuous, one has to replace the Kronecker-δ by a Dirac-δ,

$$\mathrm{d}N_{\boldsymbol{x}}(t)\mathrm{d}N_{\boldsymbol{y}}(t) = \delta\left(\boldsymbol{x}-\boldsymbol{y}\right)\mathrm{d}N_{\boldsymbol{x}}(t). \tag{2.91}$$

2.5.2. Stochastic differential equations

The Poisson process is now used to define a SDE for the trajectories of jump processes. Between two jumps, the SDE should describe a deterministic motion, whereas a discontinuous change of finite size occurs at the jump times. As a first example, consider the pure jump process in one dimension,

$$\mathrm{d}x(t) = j(x(t),t)\mathrm{d}N(t), \tag{2.92}$$

where the jump has the rate $\mathrm{E}\left[\mathrm{d}N\right]/\mathrm{d}t = \gamma(t)$. This process may describe a particle that jumps to the right by a jump width $j(x(t),t) > 0$ with rate $\gamma(t)$. The solution on the time interval $[t_0,t]$ is the stochastic trajectory $x(t)$. Since the dynamics is trivial between two jumps, i.e. nothing happens, one needs to take account for the *jump times* τ_i only, which are distributed according to the waiting-time distribution (2.80). They allow for a natural division of the interval $[t_0,t]$ into subintervals, $t_0 < \tau_1 < \cdots < \tau_n < t$. An integration of the stochastic process (2.92) is then given by a sum over the jump times τ_i,

$$x(t) = x(t_0) + \int_{t_0}^{t} j(x(t'),t')\mathrm{d}N(t') = x(t_0) + \sum_{i=1}^{n} j(x(\tau_i),\tau_i). \tag{2.93}$$

In many cases, one wants to describe a situation where the particle has different possibilities to jump to, say either to the left or to the right; even more, there can be a whole family of different jumps. In d-dimensional position space, the jumps are parametrized by their jump destination $\boldsymbol{z}$: For every possible jump one introduces an independent Poisson process $\mathrm{d}N_{\boldsymbol{z}}(t)$, which is characterized by its jump width $j_{\boldsymbol{z}}\left(\boldsymbol{x}(t),t\right) \equiv \boldsymbol{z}-\boldsymbol{x}(t)$, and occurs with a jump rate

$$\frac{\mathrm{E}\left[\mathrm{d}N_{\boldsymbol{z}}(t)\right]}{\mathrm{d}t} = W(\boldsymbol{z}|\boldsymbol{x},t). \tag{2.94}$$

By appending a drift $\boldsymbol{A}(\boldsymbol{x}(t),t)$, one obtains the corresponding SDE for this process,

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{A}(\boldsymbol{x}(t),t)\mathrm{d}t + \int \mathrm{d}\boldsymbol{z}\left[\boldsymbol{z}-\boldsymbol{x}(t)\right]\mathrm{d}N_{\boldsymbol{z}}(t), \tag{2.95}$$

where the integration goes over $\boldsymbol{z}$. As we know from the Poisson rule (2.91), there is never more than one jump at a time, which again allows for a division of the time

interval $[t_0, t]$ into subintervals built by the sequence of all waiting times τ_i of the Poisson processes $\mathrm{d}N_{\boldsymbol{z}}(t)$. It is thus straightforward to define the stochastic integral for the SDE (2.95) as well. As solution, one gets

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_0) + \int_{t_0}^{t} \mathrm{d}t' \, \boldsymbol{A}(\boldsymbol{x}(t'), t') + \int \mathrm{d}\boldsymbol{z} \int_{t_0}^{t} \mathrm{d}N_{\boldsymbol{z}}(t') \left[\boldsymbol{z} - \boldsymbol{x}(t')\right], \tag{2.96}$$

Here, the stochastic integral is given by the sum

$$\int \mathrm{d}\boldsymbol{z} \int_{t_0}^{t} \mathrm{d}N_{\boldsymbol{z}}(t') \left[\boldsymbol{z} - \boldsymbol{x}(t')\right] = \sum_{i=1}^{n} \left[\boldsymbol{z}_i - \boldsymbol{x}(\tau_i)\right], \tag{2.97}$$

where every waiting time τ_i belongs to exactly one jump with parameter $\boldsymbol{z}_i$.

Connection to jump master equation The ensemble of piecewise deterministic trajectories, which is described by the SDE (2.95) leads to a jump master equation (2.24). For simplicity, I restrict myself to the one-dimensional case and drop the time variable, i.e. $x = x(t)$ and $\mathrm{d}N_z = \mathrm{d}N_z(t)$. As in the analogous calculation for the Wiener process given in Section 2.3.3, one evaluates the time evolution of the ensemble average of an arbitrary function $f(x)$. Unlike the Wiener case, where a second order expansion in $\mathrm{d}W$ was sufficient, it is now neccessary to expand $f(x)$ to infinite order in the stochastic term

$$\mathrm{d}J(x) = \int \mathrm{d}z \, (z - x) \, \mathrm{d}N_z, \tag{2.98}$$

because of the finite jump size. One derives

$$\begin{aligned} \mathrm{d}f(x) &= f(x + \mathrm{d}x) - f(x) \\ &= f\left(x + A(x,t)\mathrm{d}t + \mathrm{d}J(x,t)\right) - f(x) \\ &= A(x,t)\frac{\partial f(x)}{\partial x}\mathrm{d}t + \sum_{n=1}^{\infty} \frac{\partial^n f(x)}{\partial x^n} \frac{[\mathrm{d}J(x,t)]^n}{n!}. \end{aligned} \tag{2.99}$$

The powers of the jump term in Eq. (2.99), are rewritten with the help of the Poisson rule (2.91) and one gets

$$[\mathrm{d}J(x,t)]^n = \left(\int \mathrm{d}z \, (z - x) \, \mathrm{d}N_z\right)^n = \int \mathrm{d}z \, (z - x)^n \, \mathrm{d}N_z, \tag{2.100}$$

which allows one to express the Taylor expansion of the jump term in Eq. (2.99) as $\int \mathrm{d}z \, [f(z) - f(x)] \, \mathrm{d}N_z$. Taking the ensemble average then yields

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}\left[f(x)\right] &\equiv \frac{1}{\mathrm{d}t}\mathrm{E}\left[\mathrm{d}f(x)\right] \\ &= \frac{1}{\mathrm{d}t}\mathrm{E}\left[A(x,t)\frac{\partial f(x)}{\partial x}\mathrm{d}t + \int \mathrm{d}z \left[f(z) - f(x)\right] \mathrm{d}N_z\right] \\ &= \mathrm{E}\left[A(x,t)\frac{\partial f(x)}{\partial x} + \int \mathrm{d}z \left[f(z) - f(x)\right] W(z|x,t)\right], \end{aligned} \tag{2.101}$$

where in the third line, I use that $f(x)$ is a non-anticipating function and therefore the ensemble average can be factorized and the Poisson increments may be replaced by their ensemble values $W(z|x,t)$, see Eq. (2.94). In the same way as for the Wiener process, an evolution equation for the probability density $p(x,t|x_0,t_0)$ is derived, which reads

$$\begin{aligned}\frac{\partial}{\partial t}p(x,t|x_0,t_0) = &-\frac{\partial}{\partial x}\left[A(x,t)p(x,t|x_0,t_0)\right] \\ &+\int \mathrm{d}z\, \left[W(x|z,t)p(z,t|x_0,t_0) - W(z|x,t)p(x,t|x_0,t_0)\right]. \quad (2.102)\end{aligned}$$

This is a jump master equation with drift, similar to the one described in Eq. (2.24).

2.5.3. Example: diffusive limit of a random walk

Under certain conditions, a jump process can also describe diffusive behavior as exhibited by the Wiener process. In particular, if one takes the limit of a jump process with increasing jump rates but decreasing jump widths, one can arrive at a diffusion process. This shall be demonstrated in the following.

Consider a one-dimensional random walker, jumping with equal probability either to the left or to the right. It is described by the SDE

$$\mathrm{d}x = j_x\left(\mathrm{d}N_1 - \mathrm{d}N_2\right), \quad (2.103)$$

including the two independent Poisson increments $\mathrm{d}N_1$ and $\mathrm{d}N_2$, which both have the rate

$$\frac{r}{2} = \frac{\mathrm{E}[\mathrm{d}N_1]}{\mathrm{d}t} = \frac{\mathrm{E}[\mathrm{d}N_2]}{\mathrm{d}t}. \quad (2.104)$$

Its jump width to either direction is j_x. The *diffusive limit* [41] is now characterized by the dependence of the jump rate and width on a parameter ε and by the scaling assumptions

$$\begin{aligned} r_\varepsilon &\to \infty, \\ j_{x,\varepsilon} &\to 0, \\ r_\varepsilon j_{x,\varepsilon}^2 &\to D, \end{aligned} \quad (2.105)$$

as $\varepsilon \to \infty$. One easily shows that the jump process (2.103) turns into a Wiener process with diffusion constant D in the diffusive limit, by comparing all moments of both stochastic processes. For that, one computes

$$\begin{aligned}(\mathrm{d}x_\varepsilon)^n &= j_{x,\varepsilon}^n\left(\mathrm{d}N_{1,\varepsilon} - \mathrm{d}N_{2,\varepsilon}\right)^n \\ &= j_{x,\varepsilon}^n \sum_{j=0}^{n} \binom{n}{j} \left(\mathrm{d}N_{1,\varepsilon}\right)^j \left(-\mathrm{d}N_{2,\varepsilon}\right)^{n-j} \\ &= j_{x,\varepsilon}^n\left(\mathrm{d}N_{1,\varepsilon} + (-1)^n\,\mathrm{d}N_{2,\varepsilon}\right), \quad (2.106)\end{aligned}$$

where the Poisson rule (2.90) is used in the third line. For the moments, one then gets

$$\begin{aligned} \mathrm{E}[(\mathrm{d}x_\varepsilon)^{2n-1}] &= 0, \\ \mathrm{E}[(\mathrm{d}x_\varepsilon)^{2n}] &= r_\varepsilon j_{x,\varepsilon}^{2n} \mathrm{d}t, \end{aligned} \tag{2.107}$$

with $n \geq 1$. The limit $\varepsilon \to \infty$ together with the scaling assumptions Eqs. (2.105) yields that only the second moment is nonvanishing,

$$\begin{aligned} \mathrm{E}[(\mathrm{d}x_\varepsilon)^2] &\to D\mathrm{d}t, \\ \mathrm{E}[(\mathrm{d}x_\varepsilon)^{2n+1}] &\to 0. \end{aligned} \tag{2.108}$$

Crucially, these are exactly the same ensemble averages that one obtains for the moments of the diffusive SDE

$$\mathrm{d}x' = \sqrt{D}\mathrm{d}W. \tag{2.109}$$

The moments are readily calculated with the help of the Ito rules (2.48) and (2.49) and they lead to the identification

$$\lim_{\varepsilon\to\infty} \mathrm{E}[(\mathrm{d}x_\varepsilon)^n] = \mathrm{E}[\left(\mathrm{d}x'\right)^n]. \tag{2.110}$$

Hence in the diffusive limit, the two stochastic processes are equivalent,

$$\lim_{\varepsilon\to\infty} \mathrm{d}x_\varepsilon = \mathrm{d}x'. \tag{2.111}$$

From the derivation, it is clear that it is essential for the diffusive limit to be feasible that the width and the rate of the jumps scale as in Eq. (2.105).

3. Dynamics of open quantum systems

In this chapter, I give an overview of the dynamics of open quantum system as far as it is needed in the later parts of this thesis. After some words on notation, I discuss the free Schrödinger equation as an example in Section 3.1.3 and introduce the Gaussian states in this context. The calculations in that section and especially the evaluation of Gaussian integrals are applied in a similar manner in the discussion of the quantum Brownian motion master equation, the collisional decoherence master equation (Chapters 4 and 5) and in Chapter 6 about the quantum linear Boltzmann equation.

Afterwards, Markovian open quantum systems are introduced and their general Lindblad form of the master equation is presented. I show elementary properties of a master equation with the help of the simple master equation of the damped harmonic oscillator in Section 3.3. They include dissipation and decoherence in position. The two master equations that play the major role in the main part of the thesis, namely the quantum Brownian motion and the collisional decoherence master equation are presented in Sections 3.4 and 3.5.

The last two sections of this chapter are devoted to the concept of pointer states, where those of the damped harmonic oscillator are taken as an example. Moreover, the pointer state unraveling is introduced, which connects the pointer states to the solution of the Lindblad master equation. These two concepts lay the groundwork for all following discussions of the pointer states of the discussed master equations and especially for the extraction of the pointer state trajectories of quantum Brownian motion.

3.1. Closed quantum systems

3.1.1. Some notation

State of the system The state of a closed quantum system is fully characterized by its *state vector* $|\psi\rangle$. In position representation, one gets the wave function $\psi(\boldsymbol{x}) = \langle \boldsymbol{x}|\psi\rangle$, with $|\psi(\boldsymbol{x})|^2$ denoting the probability density of the system to be found in the position interval $[\boldsymbol{x}, \boldsymbol{x} + \mathrm{d}\boldsymbol{x}]$. Similar relations hold for other, arbitrary bases, for instance, the momentum basis $|\boldsymbol{p}\rangle$.

If the problem is subject to a classical ignorance, meaning that its state is known only with a certain probability, one generalizes the concept of the state to the *density matrix*

$$\rho = \sum_{i=1}^{N} p_i |\psi_i\rangle\langle\psi_i|, \tag{3.1}$$

where p_i is the probability of the system to be in the normalized state $|\psi_i\rangle$. The state is

called *pure* if Eq. (3.1) consists of only one summand; this is equivalent to saying that the density matrix is a *projector*,[1]

$$\rho = |\psi\rangle\langle\psi| = \rho^2. \tag{3.2}$$

If more than one summand exists, the state is called a *mixed* state.

Born's rule The possible outcomes of a *measurement* of the observable $\hat{\mathsf{A}}$ in state $|\psi\rangle$ are the eigenvalues of $\hat{\mathsf{A}}$ and the state is thereby reduced to the corresponding eigenspace. In case of a discrete non-degenerate spectrum, the possible outcomes are a with $\hat{\mathsf{A}}|\psi_a\rangle = a|\psi_a\rangle$, where $|\psi_a\rangle$ is the appropriate eigenvector. The probability of obtaining the result a, provided the system is in $|\psi\rangle$ prior to the measurement, is given by [47–49]

$$\mathrm{Prob}(a|\psi) \equiv |\langle\psi_a|\psi\rangle|^2\,, \tag{3.3}$$

which is known as *Born's rule*.

3.1.2. Time evolution

The temporal evolution of the state $|\psi(t)\rangle$ describing an isolated, or closed, system is described by the *Schrödinger equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \frac{1}{\mathrm{i}\hbar}\hat{\mathsf{H}}|\psi(t)\rangle, \tag{3.4}$$

with *Hamiltonian*

$$\hat{\mathsf{H}} = \frac{\hat{\mathbf{p}}^2}{2m} + V\left(\hat{\mathbf{r}}\right), \tag{3.5}$$

where $\hat{\mathbf{p}}^2/2m$ is the kinetic and $V\left(\hat{\mathbf{r}}\right)$ the potential energy of a particle with mass m. In the following, the potential-free situation will be denoted as the *free* Schrödinger equation and the corresponding Hamiltonian is the *free* Hamiltonian consisting of the kinetic energy only. For the density matrix $\rho(t)$, one infers from the Schrödinger equation the *von-Neumann equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \frac{1}{\mathrm{i}\hbar}[\hat{\mathsf{H}}, \rho(t)], \tag{3.6}$$

with commutator $[\hat{\mathsf{A}}, \hat{\mathsf{B}}] = \hat{\mathsf{A}}\hat{\mathsf{B}} - \hat{\mathsf{B}}\hat{\mathsf{A}}$.

Formally, the solution to either evolution equations, Eqs. (3.4) and (3.6), can be written by using the *unitary time-evolution operator* $\hat{\mathsf{U}}(t, t_0)$, which maps the initial state $|\psi(t_0)\rangle$ to the time-evolved state

$$|\psi(t)\rangle = \hat{\mathsf{U}}(t, t_0)|\psi(t_0)\rangle, \tag{3.7}$$

or, in general, $\rho(t_0)$ is mapped to

$$\rho(t) = \hat{\mathsf{U}}(t, t_0)\rho(t_0)\hat{\mathsf{U}}^\dagger(t, t_0). \tag{3.8}$$

[1] A projector is a hermitian operator $\hat{\mathsf{P}}$ with the property $\hat{\mathsf{P}} = \hat{\mathsf{P}}^2$.

For Hamiltonians that do not explicitly depend on time the time-evolution operator has the simple exponential form

$$\hat{\mathsf{U}}(t,t_0) = \exp\left(-\mathrm{i}\hat{\mathsf{H}}(t-t_0)/\hbar\right). \tag{3.9}$$

3.1.3. Example: The free Schrödinger equation

As a simple but instructive example, an explicit solution of the free Schrödinger equation

$$\frac{\partial}{\partial t}\psi_t(\boldsymbol{x}) = -\frac{\mathrm{i}\hbar}{2m}\nabla^2\psi_t(\boldsymbol{x}), \tag{3.10}$$

is presented. By that, the Gaussian states are introduced and some of its properties are shown, which are of much use throughout this thesis. In particular, the calculation of expectation values of Gaussian states reduces to the calculation of Gaussian integrals.

As ansatz for the solution of Eq. (3.10), one takes the spherically symmetric Gaussian

$$\psi_t(\boldsymbol{x}) = \frac{1}{(2\pi V_{x,t})^{3/4}}\exp\left(-\frac{(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)^2}{4V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)+\frac{\mathrm{i}}{\hbar}(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)\cdot\overline{\boldsymbol{p}}_t+\mathrm{i}\varphi_t\right), \tag{3.11}$$

with variance $V_{x,t} = \langle\psi_t|\left(\hat{\mathsf{x}}_i-\overline{x}_{t,i}\right)^2|\psi_t\rangle$, covariance $C_{xp,t} = \langle\psi_t|\left(\hat{\mathsf{x}}_i-\overline{x}_{t,i}\right)\left(\hat{\mathsf{p}}_i-\overline{p}_{t,i}\right)+\text{h.c.}|\psi_t\rangle$, where $i\in\{1,2,3\}$, the expectation values of position and momentum vectors $\overline{\boldsymbol{x}}_t$ and $\overline{\boldsymbol{p}}_t$, and the time-dependent phase φ_t. By "h.c." I denote the hermitian conjugate of the summand to its left and, in general, I abbreviate expectation values by $\overline{A}_t \equiv \langle\psi_t|\hat{\mathsf{A}}|\psi_t\rangle$. Due to the spherical symmetry, the variances are the same in all cartesian components and one may take any index i to calculate them. Moreover, for readability, the time-dependence is denoted by an index t.

Variances of the Gaussian state Before checking that the ansatz (3.11) provides a solution of the Schrödinger equation, I want to establish the connection between the variances and the covariance of a Gaussian state. By using the ansatz (3.11) to calculate the second moment of the momentum,

$$\begin{aligned}\langle\boldsymbol{x}|\hat{\mathsf{p}}_i^2|\psi_t\rangle &= -\hbar^2\frac{\partial^2}{\partial x_i^2}\psi_t(\boldsymbol{x})\\ &= \hbar^2\left[\frac{1}{2V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)-\frac{(x_i-\overline{x}_{t,i})^2}{4V_{x,t}^2}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)^2\right.\\ &\quad\left.+\frac{\mathrm{i}}{\hbar}\frac{(x_i-\overline{x}_{t,i})\,\overline{p}_{t,i}}{V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)+\frac{\overline{p}_{t,i}^2}{\hbar^2}\right]\psi_t(\boldsymbol{x}),\end{aligned} \tag{3.12}$$

one straightforwardly derives the momentum variance of $\psi_t(\boldsymbol{x})$. It reads

$$\begin{aligned} V_{p,t} &= \langle\psi_t|\left(\hat{\mathsf{p}}_i - \overline{p}_{t,i}\right)^2|\psi_t\rangle = \overline{p_{t,i}^2} - \overline{p}_{t,i}^2 \\ &= \hbar^2\left(\frac{1-\frac{\mathrm{i}}{\hbar}C_{xp,t}}{2V_{x,t}} - \frac{\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)^2}{4V_{x,t}} + \frac{\overline{p}_{t,i}^2}{\hbar^2}\right) - \overline{p}_{t,i}^2 \\ &= \frac{\hbar^2 + C_{xp,t}^2}{4V_{x,t}}, \end{aligned} \tag{3.13}$$

where the expectation value $\overline{p_{t,i}^2}$ is calculated by simply evaluating Gaussian integrals. Finally, one arrives at the relation

$$4V_{x,t}V_{p,t} = \hbar^2 + C_{xp,t}^2. \tag{3.14}$$

As is well known, the momentum representation $\psi_t(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi_t\rangle = \int \mathrm{d}\boldsymbol{x}\langle\boldsymbol{p}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\psi_t\rangle$ of a Gaussian is also Gaussian, because one essentially performs the Fourier transform. Thus, the momentum representation of $\psi_t(\boldsymbol{x})$ is a Gaussian with variance calculated via Eq. (3.14).

Solution of the free Schrödinger equation One shows that the ansatz (3.11) solves the free Schrödinger equation (3.10) by evaluation of the time derivative as well as the Laplace operator of $\psi_t(\boldsymbol{x})$:

$$\begin{aligned} \frac{\partial}{\partial t}\psi_t(\boldsymbol{x}) = \Bigg[&-\frac{3\dot{V}_{x,t}}{4V_{x,t}} - \frac{(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)^2}{4V_{x,t}}\left[-\frac{\mathrm{i}}{\hbar}\dot{C}_{xp,t} - \frac{\dot{V}_{x,t}}{V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)\right] \\ &+ \frac{(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)\cdot\dot{\overline{\boldsymbol{x}}}_t}{2V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right) + \frac{\mathrm{i}}{\hbar}(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)\cdot\dot{\overline{\boldsymbol{p}}}_t - \frac{\mathrm{i}}{\hbar}\dot{\overline{\boldsymbol{x}}}_t\cdot\overline{\boldsymbol{p}}_t + \mathrm{i}\dot{\varphi}_t\Bigg]\psi_t(\boldsymbol{x}), \\ \nabla^2\psi_t(\boldsymbol{x}) = \Bigg[&-\frac{3}{2V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right) + \frac{(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)^2}{4V_{x,t}^2}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right)^2 \\ &- \frac{\mathrm{i}}{\hbar}\frac{(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)\cdot\overline{\boldsymbol{p}}_t}{V_{x,t}}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp,t}\right) - \frac{\overline{\boldsymbol{p}}_t^2}{\hbar^2}\Bigg]\psi_t(\boldsymbol{x}), \end{aligned} \tag{3.15}$$

where the dot is used as a shorthand notation for the time derivates, $\frac{\mathrm{d}}{\mathrm{d}t}f(t) \equiv \dot{f}(t)$. After plugging these into Eq. (3.10), one makes a comparison of coefficients in powers of $\boldsymbol{x}-\overline{\boldsymbol{x}}_t$. From the $(\boldsymbol{x}-\overline{\boldsymbol{x}}_t)^2$-term, one derives differential equations for the variances by considering the real and imaginary parts separately,

$$\begin{aligned} \dot{V}_{x,t} &= -\frac{C_{xp,t}}{m}, \\ \dot{C}_{xp,t} &= \frac{\dot{V}_{x,t}}{V_{x,t}}C_{xp,t} - \frac{\hbar^2 - C_{xp,t}^2}{2mV_{x,t}} = -\frac{2V_{p,t}}{m}, \end{aligned} \tag{3.16}$$

where one uses the variance relation (3.14) to get the second equality in the second line. Again, by using Eq. (3.14) one derives the differential equation for the momentum variance, $\dot{V}_{p,t} = 0$, which directly leads to the solutions

$$\begin{aligned} V_{p,t} &= V_{p,0}, \\ C_{xp,t} &= -\frac{2V_{p,0}}{m}t + C_{xp,0}, \\ V_{x,t} &= \frac{V_{p,0}}{m^2}\left(t - \frac{mC_{xp,0}}{2V_{p,0}}\right)^2 + \frac{\hbar^2}{2V_{p,0}}, \end{aligned} \tag{3.17}$$

where $V_{p,0}$, $C_{xp,0}$, and $V_{x,0}$ are the corresponding initial conditions. Of course, the initial conditions are connected via Eq. (3.14) so that only two of them can be chosen independently. A most prominent feature we now clearly see is that the Gaussian wave packet has a constant width in momentum space, whereas it spreads, i.e. it disperses, in position space. As opposed to diffusion, where the variance grows asymptotically linear with time, the variance of the free Schrödinger wave packet grows quadratically with time.

Those terms in the Schrödinger equation (3.10), which are linear in $\boldsymbol{x} - \overline{\boldsymbol{x}}_t$, give rise to the differential equations,

$$\begin{aligned} \dot{\overline{\boldsymbol{x}}}_t &= \frac{\overline{\boldsymbol{p}}_t}{m}, \\ \dot{\overline{\boldsymbol{p}}}_t &= 0, \end{aligned} \tag{3.18}$$

and imply a uniform movement of the wave packet, i.e. a propagation of $\overline{\boldsymbol{x}}_t$ with constant momentum $\overline{\boldsymbol{p}}_t \equiv \overline{\boldsymbol{p}}_0$. The remaining terms without $(\boldsymbol{x} - \overline{\boldsymbol{x}}_t)$-dependence specify the differential equation of the phase function,

$$\dot{\varphi}_t = \frac{3\hbar}{4mV_{x,t}} - \frac{\overline{\boldsymbol{p}}_0^2}{2m\hbar}. \tag{3.19}$$

3.2. Open quantum systems

3.2.1. Open system dynamics

A system is said to be an *open system* if it is in some way coupled to a sorrounding environment. The combined system, which consists of the system of interest and its environment, is then again a closed system and its evolution can thus be described by a unitary time evolution governed by the von-Neumann equation (3.6). The total state of system and environment is an element of the tensor product Hilbert space $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{S}} \otimes \mathcal{H}_{\text{E}}$, where $\mathcal{H}_{\text{S}}$ and $\mathcal{H}_{\text{E}}$ are the system's and environment's Hilbert spaces, respectively. The formal solution (3.8) of the total system dynamics is not quite helpful as it stands, since one is interested in the dynamics without the environment. For that reason, one traces over the environmental degrees of freedom in order to obtain the reduced state of the time evolved system,

$$\rho_{\text{S}}(t) = \text{Tr}_{\text{E}}\left[\hat{\text{U}}(t, t_0)\rho_{\text{tot}}(t_0)\hat{\text{U}}^\dagger(t, t_0)\right], \tag{3.20}$$

where $\hat{\mathsf{U}}(t, t_0)$ is the time-evolution operator of the total system. In general, the evolution of $\rho_{\mathrm{S}}(t)$ is not unitary but exhibits a highly complex irreversible dynamics.

Kraus representation A further characterization of the dynamics of the reduced state can be achieved if the system and the environment are *uncorrelated* at the initial time t_0, which means that the total state is initially in a product state,

$$\rho_{\mathrm{tot}}(t_0) = \rho_{\mathrm{S}}(t_0) \otimes \rho_{\mathrm{E}}(t_0). \tag{3.21}$$

Subsequently, one uses a decomposition of the environmental state into an orthonormal basis $|\phi_\alpha\rangle$, $\rho_{\mathrm{E}}(t_0) = \sum_\beta \lambda_\beta |\phi_\beta\rangle\langle\phi_\beta|$ to rewrite the system state in the *Kraus representation*

$$\rho_{\mathrm{S}}(t) = \sum_{\alpha,\beta} \hat{\mathsf{W}}_{\alpha,\beta}(t)\rho_{\mathrm{S}}(t_0)\hat{\mathsf{W}}^\dagger_{\alpha,\beta}(t), \tag{3.22}$$

with the *Kraus operators*

$$\hat{\mathsf{W}}_{\alpha,\beta}(t) \equiv \sqrt{\lambda_\beta}\langle\phi_\alpha|\hat{\mathsf{U}}(t, t_0)|\phi_\beta\rangle. \tag{3.23}$$

Since $\rho_{\mathrm{E}}(t_0)$ is of unit trace, one gets the condition $\sum_\beta \lambda_\beta = 1$ that leads to the condition

$$\sum_{\alpha,\beta} \hat{\mathsf{W}}^\dagger_{\alpha,\beta}(t)\hat{\mathsf{W}}_{\alpha,\beta}(t) = \mathbb{1}_{\mathrm{S}}. \tag{3.24}$$

Quantum dynamical maps Equation (3.22) defines a map $\rho_{\mathrm{S}}(t_0) \mapsto \rho_{\mathrm{S}}(t)$ between two density matrices and therefore serves as a motivation for the concept of a dynamical map, which is not neccessarily connected with the open system dynamics derived by tracing over a unitary evolution, cf. Eq. (3.20). In general, a mapping

$$\mathcal{M}_t : \rho_0 \mapsto \rho_t, \tag{3.25}$$

with parameter t, which is trace-preserving, convex linear, and completely positive is called a *dynamical map*. The parameter t can be interpreted as the time variable such that $\rho_t = \mathcal{M}_t[\rho_0]$ is the time evolved density matrix when starting in the initial state ρ_0. The preservation of the trace ensures that $\mathrm{Tr}[\rho_t] = 1$ and the condition of convex linearity,

$$\mathcal{M}_t[\lambda\rho_1 + (1-\lambda)\rho_2] = \lambda\mathcal{M}_t[\rho_1] + (1-\lambda)\mathcal{M}_t[\rho_2], \quad \text{for } \lambda \in [0,1], \tag{3.26}$$

leads to a consistent evolution of the two states, ρ_1 and ρ_2, and of a probabilistic combination therof, $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$. Finally, the third property of a dynamical map, the complete positivity, ensures for one thing that $\rho_t = \mathcal{M}_t[\rho_0]$ is positive. For another thing, if the system is part of an enlarged system, exemplified by the product of the system Hilbert space and an auxillary Hilbert space, $\mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{aux}}$, the trivially extended mapping $\mathcal{M}_t \otimes \mathbb{1}_{\mathrm{aux}}$ maps to positive states as well.

It is easily verified, that the reduced system dynamics in Eq. (3.22) in its Kraus representation has all the properties of a dynamical map. More importantly, this statement is also true in the inverse direction: A dynamical map (3.25) can always be written in the Kraus representation, which, in turn, can be understood as a reduced system dynamics of a unitary evolution [42, 50].

Quantum dynamical semigroups A dynamical map $\mathcal{M}_t$ is called a *dynamical semigroup* if it fulfills the composition rule

$$\mathcal{M}_t \mathcal{M}_u = \mathcal{M}_{t+u}, \tag{3.27}$$

for all $t, u > 0$. This property corresponds to the Markov property, which states that the dynamics of the system depends only on the present state but not on its history. For being a regular group, in general, $\mathcal{M}_t$ lacks the existence of an inverse, which would require negative time arguments and reflects that the dynamics described by semigroup mappings is irreversible and non-unitary.

By exploiting the semigroup property (3.27), one can derive a differential equation for the temporal evolution of the system state ρ_t,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = \lim_{\epsilon \to 0} \frac{1}{\varepsilon} \left(\mathcal{M}_{t+\varepsilon} \left[\rho_0\right] - \mathcal{M}_t \left[\rho_0\right] \right) = \lim_{\epsilon \to 0} \frac{1}{\varepsilon} \left(\mathcal{M}_\varepsilon - \mathbb{1}_\mathrm{S} \right) \left[\rho_t\right] \equiv \mathcal{L} \left[\rho_t\right], \tag{3.28}$$

where the super-operator $\mathcal{L}$ is called the *generator* of the dynamics. Here, we see the Markov property directly by the fact that $\mathcal{L}$ neither depends on time nor on the state; thus the dynamics of ρ_t is completely determined by its present state irrespective of its history.

3.2.2. Lindblad master equation

The most general form of the generator of a quantum dynamical semigroup is given by the Markovian master equation of *Lindblad form* [42, 51, 52]

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathcal{L}[\rho] = \frac{1}{\mathrm{i}\hbar} \left[\hat{\mathsf{H}}, \rho\right] + \mathcal{D}[\rho], \tag{3.29}$$

with $\rho \equiv \rho(t)$. The Lindblad generator $\mathcal{L}$ consists of the Hamiltonian part $\left[\hat{\mathsf{H}}, \rho\right]/\mathrm{i}\hbar$, which describes unitary evolution, and of the *dissipator*

$$\mathcal{D}[\rho] = \sum_i \gamma_i \left(\hat{\mathsf{L}}_i \rho \hat{\mathsf{L}}_i^\dagger - \frac{1}{2} \left\{ \hat{\mathsf{L}}_i^\dagger \hat{\mathsf{L}}_i, \rho \right\} \right), \tag{3.30}$$

describing the non-unitary irreversible evolution, with anticommutator $\left\{\hat{\mathsf{A}}, \hat{\mathsf{B}}\right\} = \hat{\mathsf{A}}\hat{\mathsf{B}} + \hat{\mathsf{B}}\hat{\mathsf{A}}$. A derivation of the generator (3.29) and, in particular, its dissipator (3.30) is given in Appendix B.1. The sum goes over a discrete set of dimensionless Lindblad operators $\hat{\mathsf{L}}_i$ with corresponding positive rates γ_i. For a continuous set of Lindblad operators, it has to be changed into an integral accordingly. In general, the hermitian operator $\hat{\mathsf{H}}$ differs from the free Hamiltonian of the reduced system as it may contain additional terms due to the environmental coupling.

Invariance properties of the Lindblad equation Crucially, the Lindblad operators in the dissipator Eq. (3.30) are not defined uniquely. There are symmetry transformations of the $\hat{\mathsf{L}}_i$ that leave the master equation (3.29) invariant.

First, it can be seen that the master equation is invariant under translations of the Lindblad operators by complex numbers c_i,

$$\hat{\mathsf{L}}_i' = \hat{\mathsf{L}}_i + \mathbb{1} c_i \tag{3.31}$$

if the Hamiltonian is transformed accordingly,

$$\hat{\mathsf{H}}' = \hat{\mathsf{H}} + \frac{\mathrm{i}\hbar}{2} \sum_i \gamma_i \left(c_i \hat{\mathsf{L}}_i^\dagger - c_i^* \hat{\mathsf{L}}_i \right). \tag{3.32}$$

Calculation of the translated dissipator (3.30) gives

$$\begin{aligned} \mathcal{D}'[\rho] &= \mathcal{D}[\rho] + \sum_i \gamma_i \left(\hat{\mathsf{L}}_i \rho c_i^* + c_i \rho \hat{\mathsf{L}}_i^\dagger + c_i \rho c_i^* - \frac{1}{2} \left\{ \hat{\mathsf{L}}_i^\dagger c_i + c_i^* \hat{\mathsf{L}}_i + |c_i|^2, \rho \right\} \right) \\ &= \mathcal{D}[\rho] - \sum_i \frac{\gamma_i}{2} \left(c_i \left[\hat{\mathsf{L}}_i^\dagger, \rho \right] - c_i^* \left[\hat{\mathsf{L}}_i, \rho \right] \right). \end{aligned} \tag{3.33}$$

Together with $\hat{\mathsf{H}}'$ from Eq. (3.32), one then obtains

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar} \left[\hat{\mathsf{H}}, \rho \right] + \mathcal{D}[\rho] = \frac{1}{\mathrm{i}\hbar} \left[\hat{\mathsf{H}}', \rho \right] + \mathcal{D}'[\rho]. \tag{3.34}$$

Another invariance is exploited by transforming the Lindblad operators with a unitary matrix u_{ij},

$$\sqrt{\gamma_i'} \hat{\mathsf{L}}_i' = \sum_j u_{ij} \sqrt{\gamma_j} \hat{\mathsf{L}}_j. \tag{3.35}$$

The calculation of the transformed dissipator, obtained via Eq. (3.30), yields for its first summand,

$$\sum_i \gamma_i' \hat{\mathsf{L}}_i' \rho \hat{\mathsf{L}}_i'^\dagger = \sum_{i,j,k} \sqrt{\gamma_j \gamma_k} u_{ij} u_{ik}^* \hat{\mathsf{L}}_j \rho \hat{\mathsf{L}}_k^\dagger = \sum_i \gamma_i \hat{\mathsf{L}}_i \rho \hat{\mathsf{L}}_i^\dagger, \tag{3.36}$$

where the unitarity $\sum_i u_{ik}^* u_{ij} = \delta_{jk}$ is used. Similarly, the second summand of the dissipator is also invariant, which confirms the invariance of the whole master equation (3.29). For a continuous set of Lindblad operators $\hat{\mathsf{L}}(\boldsymbol{q})$, this invariance transformation can be written as a Fourier transform

$$\sqrt{\gamma'(\boldsymbol{y})} \hat{\mathsf{L}}'(\boldsymbol{y}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \mathrm{d}\boldsymbol{q}\, \mathrm{e}^{\mathrm{i}\boldsymbol{y}\cdot\boldsymbol{q}/\hbar} \sqrt{\gamma(\boldsymbol{q})} \hat{\mathsf{L}}(\boldsymbol{q}). \tag{3.37}$$

Non-dimensionless Lindblad operators As we have already seen in the previous paragraph, it is sometimes useful to absorb the rate γ_i into the Lindblad operator,

$$\hat{\mathsf{L}}_i \to \sqrt{\gamma_i}\hat{\mathsf{L}}_i. \tag{3.38}$$

The ensuing master equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathcal{L}[\rho] = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}, \rho\right] + \sum_i \left(\hat{\mathsf{L}}_i \rho \hat{\mathsf{L}}_i^\dagger - \frac{1}{2}\left\{\hat{\mathsf{L}}_i^\dagger \hat{\mathsf{L}}_i, \rho\right\}\right), \tag{3.39}$$

with its only difference with respect to Eqs. (3.29) and (3.30) being that no γ_i appears in the equation and that the Lindblad operators have the dimension of the square-root of a rate. In most of the derivations that follow, I use this form of the master equation.

In the following three sections, I introduce Lindblad master equations that are important in the present work.

3.3. The damped harmonic oscillator

3.3.1. Master equation

The following example of the damped harmonic oscillator proves helpful in introducing the concept of pointer states in Section 3.6. Its Lindblad master equation can be obtained as the zero temperature limit, $T \to 0$, of a harmonic oscillator that is linearly coupled to a thermal bath of harmonic oscillators. Alternatively, one may prescribe the Hamiltonian $\hat{\mathsf{H}} = \hbar\omega\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}$ and the single Lindblad operator $\hat{\mathsf{L}} = \hat{\mathsf{a}}$ with rate γ, the latter mediating the incoherent evolution due to the environmental coupling. From the general Lindblad form (3.29), one then gets [53]

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\mathrm{i}\omega\left[\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}, \rho\right] + \gamma\left(\hat{\mathsf{a}}\rho\hat{\mathsf{a}}^\dagger - \frac{1}{2}\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}\rho - \frac{1}{2}\rho\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}\right). \tag{3.40}$$

Here, ω and γ denote the oscillator frequency and the damping constant and the creation and annihilation operators $\hat{\mathsf{a}}^\dagger$ and $\hat{\mathsf{a}}$ fulfill the commutation relation

$$\left[\hat{\mathsf{a}}, \hat{\mathsf{a}}^\dagger\right] = 1. \tag{3.41}$$

With the help of $\hat{\mathsf{a}}$ and $\hat{\mathsf{a}}^\dagger$, one can write the position and momentum operators of the damped harmonic oscillator [47] as

$$\begin{aligned}\hat{\mathsf{x}} &= \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{\mathsf{a}} + \hat{\mathsf{a}}^\dagger\right),\\ \hat{\mathsf{p}} &= -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{\mathsf{a}} - \hat{\mathsf{a}}^\dagger\right).\end{aligned} \tag{3.42}$$

3.3.2. Solution of the master equation

As ansatz for the solution of the damped harmonic oscillator master equation, one takes the coherent states. These are defined as eigenstates of the annihilation operator, $\hat{\mathsf{a}}|\alpha_t\rangle = \alpha_t|\alpha_t\rangle$,

$$|\alpha_t\rangle = \exp\left(-\frac{\gamma_+}{\gamma}|\alpha_t|^2 + \alpha_t\hat{\mathsf{a}}^\dagger\right)|0\rangle, \tag{3.43}$$

with $\gamma_+ = \gamma/2+\mathrm{i}\omega$. By insertion of the projector $\hat{\mathsf{P}}_\alpha = |\alpha_t\rangle\langle\alpha_t|$ into the master equation (3.40), one derives

$$\left(-2\frac{\gamma_+}{\gamma}|\alpha_t|\frac{\mathrm{d}}{\mathrm{d}t}|\alpha_t| + \hat{\mathsf{a}}^\dagger\frac{\mathrm{d}}{\mathrm{d}t}\alpha_t\right)\hat{\mathsf{P}}_\alpha + \mathrm{h.c.} = \gamma|\alpha_t|^2\hat{\mathsf{P}}_\alpha - \left(\gamma_+\alpha_t\hat{\mathsf{a}}^\dagger\hat{\mathsf{P}}_\alpha + \gamma_+^*\alpha_t^*\hat{\mathsf{P}}_\alpha\hat{\mathsf{a}}\right). \tag{3.44}$$

Setting the parameter

$$\alpha_t = \alpha_0\mathrm{e}^{-\gamma_+ t}, \tag{3.45}$$

with $\alpha_0 \in \mathbb{C}$, one easily checks that the coherent states (3.43) are indeed a solution of the damped harmonic oscillator.

The form of the coherent states can now be further investigated by calculating their first moments and their variances. For the position operator, one derives with the help of Eqs. (3.41) and (3.42),

$$\begin{aligned}\overline{x}_\alpha &= \langle\alpha_t|\hat{\mathsf{x}}|\alpha_t\rangle = \sqrt{\frac{\hbar}{2m\omega}}2\mathrm{Re}\left\{\alpha_t\right\},\\ \overline{x_\alpha^2} &= \langle\alpha_t|\hat{\mathsf{x}}^2|\alpha_t\rangle = \frac{\hbar}{2m\omega} + \overline{x}_\alpha^2.\end{aligned} \tag{3.46}$$

Thus, the position expectation undergoes a damped oscillation, which can be seen most easily from Eq. (3.45), by considering real α_0. For the momentum operator, the same calculation gives

$$\begin{aligned}\overline{p}_\alpha &= \langle\alpha_t|\hat{\mathsf{p}}|\alpha_t\rangle = \sqrt{\frac{\hbar m\omega}{2}}2\mathrm{Im}\left\{\alpha_t\right\},\\ \overline{p_\alpha^2} &= \langle\alpha_t|\hat{\mathsf{p}}^2|\alpha_t\rangle = \frac{\hbar m\omega}{2} + \overline{p}_\alpha^2,\end{aligned} \tag{3.47}$$

from which one arrives at the variances for position and momentum,

$$\begin{aligned}V_x &= \frac{\hbar}{2m\omega},\\ V_p &= \frac{\hbar m\omega}{2}.\end{aligned} \tag{3.48}$$

Finally, in position representation, the coherent states are Gaussian wave packets with constant variance V_x [47],

$$\langle x|\alpha_t\rangle = \frac{\mathrm{e}^{\mathrm{i}\phi_\alpha}}{(2\pi V_x)^{1/4}}\exp\left(-\frac{(x-\overline{x}_\alpha)^2}{4V_x} + \frac{\mathrm{i}}{\hbar}x\overline{p}_\alpha\right), \tag{3.49}$$

where the phase factor is defined by $\exp\left(\mathrm{i}\phi_\alpha\right) = \exp\left[\left(\alpha_t^{*2} - \alpha_t^2\right)/4\right]$.

Energy dissipation The expectation value of the energy of the system is readily calculated and gives

$$\overline{E}(t) = \langle\alpha_t|\hat{\mathsf{H}}|\alpha_t\rangle = \hbar\omega\langle\alpha_t|\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}|\alpha_t\rangle = \hbar\omega\,|\alpha_t|^2 = \hbar\omega\,|\alpha_0|^2\,\mathrm{e}^{-\gamma t}, \tag{3.50}$$

which shows that the system dissipates energy with an exponential decay rate γ.

3.3.3. Decoherence in position

To investigate the decoherence dynamics of the master equation, a superposition of two coherent states $|\alpha_0\rangle$ and $|\beta_0\rangle$ is considered,

$$|\psi_0\rangle = c_1|\alpha_0\rangle + c_2|\beta_0\rangle. \tag{3.51}$$

The overlap $\langle\alpha_0|\beta_0\rangle$, though never exactly vanishing, can be chosen arbitrarily small by setting $|\alpha_0 - \beta_0| \gg 1$, which corresponds to a large distance $|\overline{x}_\alpha - \overline{x}_\beta|$ of the Gaussians (3.49) with respect to their width $\sqrt{V_x}$. The associated initial density matrix has the form

$$\rho_0 = |c_1|^2\,|\alpha_0\rangle\langle\alpha_0| + |c_2|^2\,|\beta_0\rangle\langle\beta_0| + c_1c_2^*|\alpha_0\rangle\langle\beta_0| + c_1^*c_2|\beta_0\rangle\langle\alpha_0|, \tag{3.52}$$

and its time evolved counterpart reads [42, 54]

$$\rho_t = |c_1|^2\,|\alpha_t\rangle\langle\alpha_t| + |c_2|^2\,|\beta_t\rangle\langle\beta_t| + c_1c_2^*f(t)|\alpha_t\rangle\langle\beta_t| + c_1^*c_2f^*(t)|\beta_t\rangle\langle\alpha_t|. \tag{3.53}$$

The parameters α_t and β_t of the coherent states are given by Eq. (3.45) and

$$f(t) = \exp\left[\left(1 - \mathrm{e}^{-\gamma t}\right)\left(-\frac{1}{2}\,|\alpha_0 - \beta_0|^2 + \mathrm{i}\mathrm{Im}\left\{\alpha_0\beta_0^*\right\}\right)\right]. \tag{3.54}$$

For times that are short compared to the dissipative time scale, $t \ll \gamma^{-1}$, one then obtains

$$|f(t)| \approx \mathrm{e}^{-|\alpha_0-\beta_0|^2\gamma t/2}, \tag{3.55}$$

which shows that coherences are exponentially suppressed with a rate proportional to the squared distance of the coherent states [54]. By increasing the distance between the superposed wave packets, one can realize decoherence rates much greater than the dissipative rate γ. Moreover, this quadratic dependence of the decoherence rate is a general feature of models with linear environmental coupling [12] and it was also confirmed by photon cavity experiments [55].

3.4. Quantum Brownian motion

A paradigm of open quantum dynamics is the model of *quantum Brownian motion* (QBM). One method to microscopically derive dissipative dynamics is to consider a free heavy particle linearly coupled to an ideal gaseous environment. Among the first to examine this, were Caldeira and Leggett who applied a path-integral approach to trace out the environmental degrees of freedom. In the high-temperature limit they derive

the Caldeira–Leggett master equation for the reduced particle dynamics [26–29, 32, 42]. This master equation is not completely positive and thus does not have Lindblad form. The QBM master equation, which I want to consider here, can be understood as the Lindblad extension of the Caldeira–Leggett master equation. Both equations are equal except that the former has an extra term that ensures its complete positivity [32–34, 42]. It is also possible to arrive at the QBM master equation when starting with the much more general quantum linear Boltzmann equation [25] and taking the limit of a very massive particle whose state is close to thermal, see Chapter 6.

3.4.1. Master equation

The Lindblad master equation of QBM reads [34, 42]

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m},\rho\right] + \sum_{i=1}^{3}\left(\frac{\gamma}{\mathrm{i}\hbar}\left[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\rho\}\right] - \frac{2m\gamma k_\mathrm{B}T_\mathrm{env}}{\hbar^2}\left[\hat{\mathsf{x}}_i,[\hat{\mathsf{x}}_i,\rho]\right] - \frac{\gamma}{8mk_\mathrm{B}T_\mathrm{env}}\left[\hat{\mathsf{p}}_i,[\hat{\mathsf{p}}_i,\rho]\right]\right), \tag{3.56}$$

with particle mass m, friction coefficient γ, and environmental temperature T_env. Equation (3.56) is obtained from the general Lindblad form (3.39) by using the Hamiltonian

$$\hat{\mathsf{H}} = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{\gamma}{2}\sum_{i=1}^{3}\{\hat{\mathsf{x}}_i,\hat{\mathsf{p}}_i\}, \tag{3.57}$$

and the three Lindblad operators

$$\hat{\mathsf{L}}_i = \sqrt{\frac{4m\gamma k_\mathrm{B}T_\mathrm{env}}{\hbar^2}}\hat{\mathsf{x}}_i + \mathrm{i}\sqrt{\frac{\gamma}{4mk_\mathrm{B}T_\mathrm{env}}}\hat{\mathsf{p}}_i. \tag{3.58}$$

The Hamiltonian consists of the free kinetic energy of the marker particle plus an anticommutator term, which represents an energy correction due to the environmental coupling.

The first three terms in Eq. (3.56) describe free motion of the Brownian particle, its friction due to the environment, and a momentum diffusion, respectively. They constitute the Caldeira–Leggett master equation that was mentioned earlier. The fourth and last term constitutes the extra term ensuring complete positivity, i.e. it makes the master equation of Lindblad-type. Analogous to the momentum diffusion term this extra term can be identified with a position diffusion.

3.4.2. One-dimensional version

To simplify the discussion of the master equation I consider the one-dimensional version of QBM,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\frac{\hat{\mathsf{p}}^2}{2m},\rho\right] + \frac{\gamma}{\mathrm{i}\hbar}\left[\hat{\mathsf{x}},\{\hat{\mathsf{p}},\rho\}\right] - \frac{2m\gamma k_\mathrm{B}T_\mathrm{env}}{\hbar^2}\left[\hat{\mathsf{x}},[\hat{\mathsf{x}},\rho]\right] - \frac{\gamma}{8mk_\mathrm{B}T_\mathrm{env}}\left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\rho]\right]. \tag{3.59}$$

Notice that one can construct solutions of the higher-dimensional QBM master equation (3.56) from solutions of the 1D form (3.59). In particular, from two solutions ρ_1 and ρ_2 of the 1D QBM (3.59) one gets a solution for the 2D QBM by the product $\rho = \rho_1 \otimes \rho_2$. Obviously, the 2D QBM is obtained from Eq. (3.56) by summing only up to 2. Calculation of the time derivative of the product state gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{\mathrm{d}}{\mathrm{d}t}\rho_1 \otimes \rho_2 + \rho_1 \otimes \frac{\mathrm{d}}{\mathrm{d}t}\rho_2, \tag{3.60}$$

and inserting Eq. (3.59) yields the 2D version of QBM. Solutions in three dimensions are constructed accordingly.

However, one should keep in mind that in addition to the solutions which are of product form, $\rho = \rho_1 \otimes \rho_2 \otimes \rho_3$, there may be as well solutions of the 3D master equation which cannot be factorized into 1D solutions. Nonetheless, a great deal of QBM is captured by considering the 1D case only, as I do in the following.

3.4.3. Dimensionless form

For convenience, I choose dimensionless variables by introducing time, length, and momentum scales. In order to be valuable in drawing the semiclassical limit of QBM, these scales should be interpretable with classical terms only and therefore should not involve $\hbar$. One possibility is given by

$$\mathrm{T} = \frac{1}{2\gamma}, \quad \mathrm{L} = \frac{1}{2\gamma}\sqrt{\frac{k_\mathrm{B}T_\mathrm{env}}{m}}, \quad \mathrm{P} = \sqrt{mk_\mathrm{B}T_\mathrm{env}}, \tag{3.61}$$

where T is choosen according to the natural classical time scale given by the inverse friction constant and the momentum scale P is defined by the equipartition theorem. The length scale is then fixed by requiring $\mathrm{P} = m\mathrm{L}/\mathrm{T}$. The dimensionless Hamiltonian and the Lindblad operator are then obtained from the 1D forms of Eqs. (3.57) and (3.58),

$$\begin{aligned} \hat{\mathsf{H}} &= \kappa\left(\frac{\hat{\mathsf{p}}^2}{2} + \frac{1}{4}\left\{\hat{\mathsf{x}},\hat{\mathsf{p}}\right\}\right), \\ \hat{\mathsf{L}} &= \sqrt{2}\left(\kappa\hat{\mathsf{x}} + \frac{\mathrm{i}}{4}\hat{\mathsf{p}}\right). \end{aligned} \tag{3.62}$$

They lead to the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{p}}^2,\rho\right] - \mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{x}},\{\hat{\mathsf{p}},\rho\}\right] - \kappa^2\left[\hat{\mathsf{x}},[\hat{\mathsf{x}},\rho]\right] - \frac{1}{16}\left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\rho]\right], \tag{3.63}$$

where I introduced the dimensionless parameter

$$\kappa \equiv \frac{k_\mathrm{B}T_\mathrm{env}}{2\gamma\hbar}. \tag{3.64}$$

In these dimensionless units, the commutator between position and momentum operator reads

$$[\hat{\mathsf{x}},\hat{\mathsf{p}}] = \left[\frac{\hat{\mathsf{x}}_\mathrm{phys}}{\mathrm{L}},\frac{\hat{\mathsf{p}}_\mathrm{phys}}{\mathrm{P}}\right] = \frac{\mathrm{i}2\gamma\hbar}{k_\mathrm{B}T_\mathrm{env}} = \frac{i}{\kappa}, \tag{3.65}$$

with $\hat{\mathsf{x}}_{\mathrm{phys}}$ and $\hat{\mathsf{p}}_{\mathrm{phys}}$ denoting the position and momentum operator in physical units. Analogously, one derives the position representation of the momentum operator,

$$\langle x|\hat{\mathsf{p}}|\Phi\rangle = -\frac{\mathrm{i}}{\kappa}\frac{\partial}{\partial x}\Phi(x). \tag{3.66}$$

The *semiclassical limit*, which I use to describe classical behavior emerging from QBM, is normally said to be the limit of vanishing $\hbar$; in the present case this corresponds to sending the dimensionless parameter $\kappa \to \infty$. The influence of the position diffusion term, i.e. the last term in Eq. (3.63), which distinguishes the QBM master equation from the Caldeira–Leggett master equation, becomes weaker as κ grows. In fact, in the semiclassical regime, only the friction and the momentum diffusion terms are relevant in the dissipator.

3.4.4. Decoherence in position

At first, it shall be shown that the QBM master equation leads to spatial decoherence. By switching to the interaction picture,

$$\tilde{\rho} = \mathrm{e}^{\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}\rho\mathrm{e}^{-\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}, \tag{3.67}$$

with free Hamiltonian $\hat{\mathsf{H}}_0 = \kappa\hat{\mathsf{p}}^2/2$, the master equation in position representation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x|\tilde{\rho}|x'\rangle = \left[\frac{1}{2}\left(x-x'\right)\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right) - \kappa^2\left(x-x'\right)^2 + \frac{1}{16\kappa^2}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)^2\right]\langle x|\tilde{\rho}|x'\rangle. \tag{3.68}$$

For large κ, the second term on the right-hand side is the dominant one as it grows quadratically with κ. Equation (3.68) then simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x|\tilde{\rho}|x'\rangle \approx -\kappa^2\left(x-x'\right)^2\langle x|\tilde{\rho}|x'\rangle, \tag{3.69}$$

which is solved by exponentially decaying coherences,

$$\langle x|\tilde{\rho}|x'\rangle(t) = \mathrm{e}^{-F(x-x')t}\langle x|\tilde{\rho}|x'\rangle(0), \tag{3.70}$$

with *localization rate*

$$F(s) = \kappa^2 s^2. \tag{3.71}$$

Like for the damped harmonic oscillator, the localization rate grows quadratically with the distance and grows above all bounds for large s. Additionally, one sees that the influence of decoherence becomes more and more pronounced for growing κ.

3.4.5. Expectation values of the master equation

The derivation of differential equations for the first moments and the variances of the master equation allows us to explore similarities to the classical Brownian motion (CBM)

case, which was considered in Section 2.4.3. Most prominently, one sees that the position variance in the QBM master equation also involves a term that grows linearly with time.

The differential equations for the expectation values $\overline{A} = \mathrm{Tr}\left[\rho\hat{\mathsf{A}}\right]$ are calculated straightforwardly by making use of the master equation (3.63),

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{A} &= \mathrm{Tr}\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\rho\right)\hat{\mathsf{A}}\right] \\ &= \mathrm{Tr}\left[\left(-\mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{p}}^2,\rho\right] - \mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{x}},\{\hat{\mathsf{p}},\rho\}\right] - \kappa^2\left[\hat{\mathsf{x}},[\hat{\mathsf{x}},\rho]\right] - \frac{1}{16}\left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\rho]\right]\right)\hat{\mathsf{A}}\right]. \end{aligned} \tag{3.72}$$

As a first step, it is convenient to expand the terms in Eq. (3.72), which include two commutators,

$$\begin{aligned}\left[\hat{\mathsf{x}},\{\hat{\mathsf{p}},\rho\}\right] &= \hat{\mathsf{x}}\hat{\mathsf{p}}\rho + \hat{\mathsf{x}}\rho\hat{\mathsf{p}} - \hat{\mathsf{p}}\rho\hat{\mathsf{x}} - \rho\hat{\mathsf{p}}\hat{\mathsf{x}}, \\ \left[\hat{\mathsf{x}},[\hat{\mathsf{x}},\rho]\right] &= \hat{\mathsf{x}}^2\rho + \rho\hat{\mathsf{x}}^2 - 2\hat{\mathsf{x}}\rho\hat{\mathsf{x}}, \\ \left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\rho]\right] &= \hat{\mathsf{p}}^2\rho + \rho\hat{\mathsf{p}}^2 - 2\hat{\mathsf{p}}\rho\hat{\mathsf{p}}. \end{aligned} \tag{3.73}$$

Then, by making extensive use of the cyclic invariance of the trace, one directly calculates the differential equation for the position expectation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{x} = \mathrm{Tr}\left[\rho\left(-\mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{x}},\hat{\mathsf{p}}^2\right] - \frac{1}{16}\left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\hat{\mathsf{x}}]\right]\right)\right], \tag{3.74}$$

where the canonical commutator is taken from Eq. (3.65), $\left[\hat{\mathsf{x}},\hat{\mathsf{p}}\right] = \mathrm{i}/\kappa$, which allows the calculation of $\left[\hat{\mathsf{x}},\hat{\mathsf{p}}^2\right] = 2\mathrm{i}\hat{\mathsf{p}}/\kappa$. Finally, one gets

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{x} = \overline{p}. \tag{3.75}$$

For the momentum expectation, a similar derivation gives

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{p} &= \mathrm{Tr}\left[\rho\left(-\mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{p}}^2,\hat{\mathsf{x}}\right] - \kappa^2\left[\hat{\mathsf{x}},[\hat{\mathsf{x}},\hat{\mathsf{p}}]\right]\right)\right] \\ &= -\overline{p}. \end{aligned} \tag{3.76}$$

Along the same lines, the derivation of the second position moment yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{x^2} &= \mathrm{Tr}\left[\rho\left(-\mathrm{i}\frac{\kappa}{2}\left[\hat{\mathsf{x}}^2,\hat{\mathsf{p}}^2\right] - \frac{1}{16}\left[\hat{\mathsf{p}},[\hat{\mathsf{p}},\hat{\mathsf{x}}^2]\right]\right)\right] \\ &= \overline{\{x,p\}} + \frac{1}{8\kappa^2}, \end{aligned} \tag{3.77}$$

where, in the second line, I used $\left[\hat{\mathsf{x}}^2,\hat{\mathsf{p}}\right] = 2\mathrm{i}\hat{\mathsf{x}}/\kappa$ and $\left[\hat{\mathsf{x}}^2,\hat{\mathsf{p}}^2\right] = 2\mathrm{i}\left\{\hat{\mathsf{x}},\hat{\mathsf{p}}\right\}/\kappa$. Analogously, for the second moment of the momentum operator one gets

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{p^2} &= \mathrm{Tr}\left[\rho\left(-\mathrm{i}\frac{\kappa}{2}\left\{\hat{\mathsf{p}},\left[\hat{\mathsf{p}}^2,\hat{\mathsf{x}}\right]\right\} - \kappa^2\left[\hat{\mathsf{x}},\left[\hat{\mathsf{x}},\hat{\mathsf{p}}^2\right]\right]\right)\right] \\ &= -2\overline{p^2} + 2, \end{aligned} \tag{3.78}$$

and the equation of motion for the mean value $\overline{\{x,p\}}$ reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{\{x,p\}} &= \mathrm{Tr}\left[\rho\left(-\mathrm{i}\kappa\left[\hat{\mathsf{x}}\hat{\mathsf{p}},\hat{\mathsf{p}}^2\right]-\mathrm{i}\kappa\left(\hat{\mathsf{x}}\hat{\mathsf{p}}\hat{\mathsf{x}}\hat{\mathsf{p}}+\hat{\mathsf{p}}\hat{\mathsf{x}}\hat{\mathsf{p}}\hat{\mathsf{x}}-\hat{\mathsf{x}}^2\hat{\mathsf{p}}^2-\hat{\mathsf{p}}\hat{\mathsf{x}}^2\hat{\mathsf{p}}\right)\right)\right] \\ &= 2\overline{p^2}-\overline{\{x,p\}},\end{aligned} \tag{3.79}$$

where one uses that $\mathrm{Tr}\left[\mathrm{d}\rho/\mathrm{d}t\right]=0$, which leads to $\mathrm{d}\overline{\{x,p\}}/\mathrm{d}t = 2\mathrm{d}\overline{xp}/\mathrm{d}t$.

By using the equations of motion for the first and second moments, Eqs. (3.75)-(3.79), one now derives the differential equations for the variances $V_x = \overline{x^2}-\overline{x}^2$ and $V_p = \overline{p^2}-\overline{p}^2$ as well as for the covariance $C_{xp} = \overline{\{x,p\}} - 2\overline{x}\,\overline{p}$,[2]

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V_x &= C_{xp}+\frac{1}{8\kappa^2}, \\ \frac{\mathrm{d}}{\mathrm{d}t}V_p &= -2V_p+2, \\ \frac{\mathrm{d}}{\mathrm{d}t}C_{xp} &= -C_{xp}+2V_p.\end{aligned} \tag{3.80}$$

These differential equations are very similar to those of the classical phase space diffusion, see Eqs. (2.65) and (2.70) in Section 2.4. Actually, one can match both sets of equations by identifying the diffusion constants of Eqs. (2.70) as $D_x = 1/8\kappa^2$, $D_p = 2$, and $D_{xp} = 0$. Note that there is a differing factor of two between the definitions of the classical covariance $\mathrm{Cov}[x,p]$ in Eqs. (2.67) and the quantum version C_{xp}.

The solutions of Eqs. (3.75), (3.76), and (3.80) are readily obtained from the classical solutions, which are shown in Eqs. (2.66) and (2.71). Consequently, the first moments describe a motion with exponentially damped momentum, i.e. *friction*,

$$\begin{aligned}\overline{x}(t) &= \overline{x}_0+\overline{p}_0\left(1-\mathrm{e}^{-t}\right), \\ \overline{p}(t) &= \overline{p}_0\mathrm{e}^{-t},\end{aligned} \tag{3.81}$$

with initial values $\overline{x}_0$ and $\overline{p}_0$; the variances read

$$\begin{aligned}V_x(t) &= V_{x,0}+\left(V_{p,0}-1\right)\left(1-\mathrm{e}^{-t}\right)^2 \\ &\quad +\left(C_{xp,0}-2\right)\left(1-\mathrm{e}^{-t}\right)+\left(\frac{1}{8\kappa^2}+2\right)t, \\ V_p(t) &= V_{p,0}\mathrm{e}^{-2t}+1-\mathrm{e}^{-2t}, \\ C_{xp}(t) &= C_{xp,0}\mathrm{e}^{-t}+2V_{p,0}\mathrm{e}^{-t}\left(1-\mathrm{e}^{-t}\right)+2\left(1-\mathrm{e}^{-t}\right)^2,\end{aligned} \tag{3.82}$$

with the initial values $V_{x,0}$, $V_{p,0}$, and $C_{xp,0}$. As we can see, the position variance $V_x(t)$ involves a term that grows linearly with time, which indicates the *diffusive behavior* described by the QBM master equation. The two other variances $V_p(t)$ and $C_{xp}(t)$ approach stationary values for large times.

[2] A similar set of differential equations is obtained for the Caldeira–Leggett master equation and may be found in Ref. [42].

Energy dissipation The dissipation of energy and its eventual thermalization is infered directly from Eqs. (3.81) and (3.82), as the kinetic energy has the form $E(t) = \kappa\overline{p^2}(t)/2$. One gets

$$E(t) = E_0 \mathrm{e}^{-2t} + \frac{\kappa}{2}\left(1 - \mathrm{e}^{-2t}\right), \tag{3.83}$$

with initial value $E_0 = \kappa\left(V_{p,0} + \overline{p}_0^2\right)/2$. For long times, it approaches the value expected by the equipartition theorem; using physical units, $E_{\mathrm{phys}} = E\hbar/\mathrm{T}$, one evaluates $E_{\infty,\mathrm{phys}} = k_{\mathrm{B}}T_{\mathrm{env}}/2$.

3.5. Collisional decoherence

3.5.1. Master equation

The master equation of *collisional decoherence* is obtained when considering the short-time behavior of a very massive test particle in a gas environment. For short periods of time, friction and damping effects of the environment are negligible and only decoherence effects need to be described. The family of Lindblad operators, one gets from a scattering analysis, has the form [40, 56]

$$\hat{\mathsf{L}}_{\boldsymbol{q}} = \sqrt{\gamma G(\boldsymbol{q})}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar}, \tag{3.84}$$

with the normalized probability distribution $G(\boldsymbol{q})$ of momentum kicks and the total kick rate γ. These Lindblad operators describe momentum kicks and yield the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}_0, \rho\right] + \gamma\int \mathrm{d}\boldsymbol{q}\, G\left(\boldsymbol{q}\right)\left(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar}\rho\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar} - \rho\right), \tag{3.85}$$

with free Hamiltonian

$$\hat{\mathsf{H}}_0 = \frac{\hat{\mathbf{p}}^2}{2m}, \tag{3.86}$$

and particle mass m.

If one looks for the general form of a Lindblad master equation with bounded Lindblad operators, whose dissipator depends on the position operator only and which is covariant under spatial translations [57–60], one also ends up with Eq. (3.85). Interestingly, the collisional decoherence master equation can be obtained as a limit of the more general quantum linear Boltzmann equation, which describes the reduced dissipative and decoherent dynamics of a marker particle immersed in an ideal gaseous environment [25], see Section 6.2.1. In this context, one can derive the momentum transfer distribution $G\left(\boldsymbol{q}\right)$ with the help of microscopic quantities, e.g. the environmental gas density and the elastic scattering amplitude.

3.5.2. Decoherence in position

The collisional decoherence master equation leads to localized states via spatial decoherence. To see this, one goes to the interaction picture and uses the position representation

of Eq. (3.85). One gets [54]

$$\begin{aligned} \tilde{\rho} &= \mathrm{e}^{\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}\rho\mathrm{e}^{-\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle\boldsymbol{x}|\tilde{\rho}|\boldsymbol{x}'\rangle &= \gamma\int \mathrm{d}\boldsymbol{q}G\left(\boldsymbol{q}\right)\left(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}-1\right)\langle\boldsymbol{x}|\tilde{\rho}|\boldsymbol{x}'\rangle. \end{aligned} \tag{3.87}$$

The solution of this equation yields an exponential decay of the spatial coherences,

$$\langle\boldsymbol{x}|\tilde{\rho}|\boldsymbol{x}'\rangle(t) = \mathrm{e}^{-F(\boldsymbol{x}-\boldsymbol{x}')t}\langle\boldsymbol{x}|\tilde{\rho}|\boldsymbol{x}'\rangle(0), \tag{3.88}$$

with the *localization rate*

$$F\left(\boldsymbol{s}\right) = \gamma\left(1-\int \mathrm{d}\boldsymbol{q}G\left(\boldsymbol{q}\right)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}/\hbar}\right). \tag{3.89}$$

If the probability distribution $G(\boldsymbol{q})$ is assumed to be isotropic, then the localization rate $F(\boldsymbol{s})$ is real and non-negative. The non-negativity of $F(\boldsymbol{s})$ is readily seen by using the triangle inequality,

$$\left|\int \mathrm{d}\boldsymbol{q}G\left(\boldsymbol{q}\right)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}/\hbar}\right| \leq \int \mathrm{d}\boldsymbol{q}\left|G\left(\boldsymbol{q}\right)\right| = 1, \tag{3.90}$$

with $G(\boldsymbol{q})$ strictly positive and normalized. Additionally, the localization rate saturates for large spatial separations, i.e. $F(\boldsymbol{s}) \to \gamma$ for $\boldsymbol{s} \to \infty$, which is due to the highly oscillating phase factor in Eq. (3.89). In contrast to that, decoherence models based on a linear environmental coupling like the damped harmonic oscillator and QBM give rise to localization rates that increase with the squared distance $|\boldsymbol{x}-\boldsymbol{x}'|^2$ and, in particular, that do not saturate. There have been several interference experiments with fullerene molecules in accordance with a saturating localization rate [1, 61].

3.5.3. One-dimensional version

The collisional decoherence master equation (3.85) is written in its three-dimensional form. The natural analogue in one dimension is obtained by using the Lindblad operators $\hat{\mathsf{L}}_q = \sqrt{\gamma G(q)}\exp\left(\mathrm{i}q\hat{\mathsf{x}}/\hbar\right)$ and the Hamiltonian $\hat{\mathsf{H}}_0 = \hat{\mathsf{p}}^2/2m$, which leads to the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}_0,\rho\right] + \gamma\int \mathrm{d}q\, G\left(q\right)\left(\mathrm{e}^{\mathrm{i}q\hat{\mathsf{x}}/\hbar}\rho\mathrm{e}^{-\mathrm{i}q\hat{\mathsf{x}}/\hbar}-\rho\right). \tag{3.91}$$

As is confirmed easily, one *cannot* obtain solutions of the three-dimensional problem using a product ansatz of the one-dimensional solutions of Eq. (3.91). Busse and Hornberger [37–39] extensively analyzed the collisional decoherence master equation, its pointer states, and their emerging classical equations of motion in the one-dimensional case.

3.6. Pointer states

In many situations, the Lindblad master equation, which describes the evolution of an open quantum system, displays a timescale separation into a short decoherence time t_{dec} and a much longer dynamical timescale that has also a classical meaning. An example for this, which was shown in the section above, is the damped harmonic oscillator, where the longer "classical" timescale is identified with the inverse damping rate. One then expects the system to exhibit a special set of states, the so-called *pointer states* [17]. These are localized states in phase space, which are relatively stable and change on the longer timescale only. Additionally, superpositions of mutually orthogonal pointer states decay into a mixture on the short decoherence timescale.

To be specific, for an initial superposition of pointer states $|\pi_\alpha(0)\rangle$,

$$|\psi_0\rangle = \sum_\alpha c_\alpha(0)|\pi_\alpha(0)\rangle, \tag{3.92}$$

and for times much greater than the decoherence time, $t \gg t_{\mathrm{dec}}$, the solution of the master equation should be well approximated by a specific mixture of pointer states [42]

$$\rho_0 = |\psi_0\rangle\langle\psi_0| \to \rho_t \simeq \sum_\alpha \mathrm{Prob}(\alpha|\rho_0)|\pi_\alpha(t)\rangle\langle\pi_\alpha(t)|. \tag{3.93}$$

A proper set of pointer states forms a basis and is independent of the initial state. Their shape depends only on the details of the environmental coupling. The mixture (3.93) of pointer states depends on the initial state ρ_0 only via the probability distribution $\mathrm{Prob}\,(\alpha|\rho_0)$. In accordance with the Born rule (3.3), the probability of the mixture (3.93) to be in pointer state $|\pi_\alpha(t)\rangle$ should be given by the overlap of that pointer state at initial time with the inital superposition state,

$$\mathrm{Prob}(\alpha|\rho_0) = \mathrm{Tr}\,[\rho_0|\pi_\alpha(0)\rangle\langle\pi_\alpha(0)|] = |c_\alpha(0)|^2. \tag{3.94}$$

A great merit of using the pointer states is that one does not need to solve the whole master equation because its dynamics is fully captured by the much simpler Eq. (3.93) for times much greater than t_{dec}. For this, one first has to identify the shape of the pointer states and verify that their probability in the mixture is according to Eq. (3.94). Secondly, their time dependence, which occurs on the longer "classical" scale has to be identified; it constitutes a motion of the pointer states' expectation values in phase space. The result is an ensemble of localized pointer states that moves on trajectories in phase space.

There are several methods to define the pointer states of a master equation. One possibility being the *predictability sieve*, which defines the pointer states as the least entropy producing states [18, 19]. In order to find the pointer states, one may thus minimize the *linear entropy production*

$$\frac{\mathrm{d}}{\mathrm{d}t}S_{\mathrm{lin}}\,[\rho] = -2\mathrm{Tr}\left[\rho\frac{\mathrm{d}}{\mathrm{d}t}\rho\right], \tag{3.95}$$

where $S_{\mathrm{lin}}[\rho] = 1 - \mathrm{Tr}\left[\rho^2\right]$ is the so-called linear entropy. The trace of ρ^2 is unity if and only if the state is pure and less than one otherwise. Thus, $S_{\mathrm{lin}}[\rho]$ is also a measure for the purity of the state, and consequently, the predictability sieve selects those states being most robust with respect to purity.

In this work, however, the pointer states are characterized by another approach; they are identified as the soliton-like stable solutions of a nonlinear equation associated with the master equation.

3.6.1. The nonlinear pointer state equation (NLPSE)

The *nonlinear pointer state equation* (NLPSE) is a tool to identify the pointer states and it is obtained by looking for an evolution of pure states that resembles the dynamics of the master equation as closely as possible [20, 21, 39, 62, 63]. In general, the evolution due to a master equation leads to a mixed state, even if the initial state was pure. The NLPSE can be regarded as the nonlinear mapping of that mixed state onto the space of pure states. This concept may seem somewhat unmotivated at that stage, but will become clear with the introduction of an unraveling in Section 3.7. At the present point, the NLPSE is presented heuristically as one way to obtain the pointer states. The derivation of the NLPSE accompanying the Lindblad master equation (3.39) is given in Appendix B.2 and yields [21]

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{\mathsf{N}}[\psi]\,|\psi\rangle = \left[\frac{1}{\mathrm{i}\hbar}\left(\hat{\mathsf{H}} - \overline{H}\right) + \sum_i \left(\frac{1}{2}\left(\overline{L_i^\dagger L_i} - \hat{\mathsf{L}}_i^\dagger \hat{\mathsf{L}}_i\right) + \overline{L_i^\dagger}\left(\hat{\mathsf{L}}_i - \overline{L}_i\right)\right)\right]|\psi\rangle. \tag{3.96}$$

As usual, $\overline{A} \equiv \langle\psi|\hat{\mathsf{A}}|\psi\rangle$ denotes expectation values and the time dependence of the state $|\psi\rangle$ is omitted for brevity.

Those solutions $|\pi\rangle$ of the NLPSE (3.96), with a time-constant shape

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\pi(\boldsymbol{x})| = 0, \tag{3.97}$$

are called "soliton-like" solutions and they are candidates for the pointer states of the master equation. In order for them to be genuine pointer states, one has to verify all the properties stated in the previous section, for example that superpositions of these states decohere very fast and that they are stable solutions.

3.6.2. Pointer states of the damped harmonic oscillator

As an example, let us consider the pointer states of the damped harmonic oscillator, which was discussed in Section 3.3. The NLPSE follows immediately from the general form (3.96),

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \left[-\mathrm{i}\omega\left(\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}} - \overline{a^\dagger a}\right) + \gamma\left(\overline{a^\dagger}\left(\hat{\mathsf{a}} - \overline{a}\right) - \frac{1}{2}\left(\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}} - \overline{a^\dagger a}\right)\right)\right]|\psi\rangle. \tag{3.98}$$

As can be verified by a short calculation, the coherent states (3.43), being the solutions of the master equation of the damped harmonic oscillator, are also a solution of the NLPSE. Interestingly, the coherent states are not the only solutions; the Fock states $|n\rangle$, defined as the states of definite particle number, $\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}|n\rangle = n|n\rangle$, are also solutions of the NLPSE. By additionally considering the predictability sieve, one shows that only the coherent states minimize the entropy production (3.95). In particular, one derives for the coherent states

$$\frac{\mathrm{d}}{\mathrm{d}t}S_{\mathrm{lin}}\left(|\alpha_t\rangle\langle\alpha_t|\right) = -\mathrm{Tr}\left[|\alpha_t\rangle\langle\alpha_t|\mathcal{L}\left(|\alpha_t\rangle\langle\alpha_t|\right)\right] = 0, \tag{3.99}$$

whereas for the Fock states one gets

$$\frac{\mathrm{d}}{\mathrm{d}t}S_{\mathrm{lin}}\left(|n\rangle\langle n|\right) = -\mathrm{Tr}\left[|n\rangle\langle n|\mathcal{L}\left(|n\rangle\langle n|\right)\right] = 2\gamma n. \tag{3.100}$$

Although both $|\alpha_t\rangle$ and $|n\rangle$ solve the NLPSE (3.98), only the coherent states (3.43) are also selected by the predictability sieve. This suggests that they build the pointer basis of the damped harmonic oscillator.

Even without consulting the pointer state condition imposed by the predictability sieve, one nevertheless ends up with the coherent states as the pointer states, because the Fock states are unstable solutions of the NLPSE. To see this, we need to connect the dynamics of the NLPSE with that of the master equation, which is done by a so-called unraveling.

3.7. Unraveling of the master equation

The NLPSE, as introduced in the previous section, is an evolution equation that may provide the pointer states as stable soliton-like solutions. In this last section of this chapter, I draw the precise connection between the NLPSE and the Lindblad master equation. We saw in Chapter 2, that one can switch from the description of a classical Markovian process via a master equation for a probability density to a trajectory picture. In general, these trajectories are governed by stochastic differential equations and they reproduce the evolution of the master equation in the ensemble average. Similarly, in the quantum case one can replace the density matrix, which is governed by a Lindblad master equation, by quantum trajectories, which consist of pure states governed by a quantum stochastic differential equation. The ensemble of quantum trajectories then reproduces exactly the density matrix that appears as solution of the Lindblad master equation. Each such ensemble of quantum trajectories is called an *unraveling* of the master equation. Crucially, in contrast to the classical case, where an ensemble of stochastic trajectories can be connected uniquely with its probability description, the decomposition of the density matrix into a mixture (or an ensemble) of pure states is ambiguous. Consequently, there are many unravelings of a given master equation. One can distinguish between continuous unravelings based on a Wiener process [8, 31, 62, 64, 65], where *quantum state diffusion* is the most prominent, and piecewise deterministic unravelings [20, 21, 38, 39, 66, 67] based on a Poisson process.

3.7.1. Pointer state unraveling

In the present work, I use a particular Poisson based unraveling, which I call the *pointer state unraveling*. The name is due to the characterizing fact that its deterministic part is given by the NLPSE. The deterministic evolution of the accompanied quantum trajectories thus produces the pointer states and the stochastic dynamics of this unraveling leads to Poissonian distributed jumps of the wave function. The pointer state unraveling was already employed in the case of collisional decoherence to determine the pointer states and to find the phase space trajectories they move on [37–39].

The stochastic differential equation of the pointer state unraveling has the form [21, 37, 68]

$$|\mathrm{d}\psi\rangle = \hat{\mathsf{N}}\left[\psi\right]|\psi\rangle\mathrm{d}t + \sum_i \left(\frac{\hat{\mathsf{J}}_i\left[\psi\right]}{\|\hat{\mathsf{J}}_i\left[\psi\right]|\psi\rangle\|} - 1\right)|\psi\rangle\mathrm{d}N_i(t), \tag{3.101}$$

where $\hat{\mathsf{N}}\left[\psi\right]$ is the nonlinear operator of the NLPSE (3.96) and the $\hat{\mathsf{J}}_i\left[\psi\right]$ are called the *jump operators*. In general, I denote a nonlinear operator by a square bracket following the operator symbol. For a continuous set of jumps, the sum in Eq. (3.101) has to be replaced by the appropriate integral, completely analogous as for the Lindblad master equation (3.39). The nonlinear jump operators are connected to the Lindblad operators,

$$\hat{\mathsf{J}}_i\left[\psi\right] = \hat{\mathsf{L}}_i - \overline{L}_i, \tag{3.102}$$

defining jumps with mutually independent Poisson increments $\mathrm{d}N_i(t)$. The Poisson increments are introduced in Section 2.5 and follow the Poisson rule (2.90). According to Eq. (3.101), a jump with index i causes the state transformation $|\psi\rangle \longrightarrow \hat{\mathsf{J}}_i\left[\psi\right]|\psi\rangle/\mathcal{N}$, where $\mathcal{N}$ denotes the normalization constant. It is easily seen that the state directly after the jump is orthogonal to the state before the jump; that is why this unraveling is sometimes called the *orthogonal unraveling* [37–39, 68]: $\langle\psi|\hat{\mathsf{J}}_i\left[\psi\right]|\psi\rangle = \langle\psi|\hat{\mathsf{L}}_i - \overline{L}_i|\psi\rangle = 0$.

The jump rates of the Poisson processes are given by

$$r_i = \frac{\mathrm{E}\left[\mathrm{d}N_i(t)\right]}{\mathrm{d}t} = \langle\psi|\hat{\mathsf{J}}_i^\dagger\left[\psi\right]\hat{\mathsf{J}}_i\left[\psi\right]|\psi\rangle = \overline{L_i^\dagger L_i} - \overline{L_i^\dagger}\,\overline{L_i}. \tag{3.103}$$

These rates are time- and state-dependent due to the occurence of expectation values including the state $|\psi\rangle$, which depends on time in general.

Diffusive unravelings Just to mention, the most prominent continuous stochastic unraveling, called quantum state diffusion, is based on a Wiener process and its Ito form is given by [65, 69]

$$|\mathrm{d}\psi\rangle = \left[\frac{1}{\mathrm{i}\hbar}\hat{\mathsf{H}} + \sum_i\left(\overline{L_i^\dagger}\hat{\mathsf{L}}_i - \frac{1}{2}\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i - \frac{1}{2}\overline{L}_i^\dagger\overline{L}_i\right)\right]|\psi\rangle\mathrm{d}t + \sum_i\left(\hat{\mathsf{L}}_i - \overline{L}_i\right)|\psi\rangle\mathrm{d}W_i(t), \tag{3.104}$$

where the $\mathrm{d}W_i(t)$ represent independent, normalized complex Wiener increments. It is a notable coincidence that its deterministic part is exactly the NLPSE (3.96) when

rewriting this Ito stochastic differential equation in its corresponding Stratonovich form [68].

3.7.2. Ensemble average

One needs to check that the pointer state unraveling, given in Eq. (3.101), reproduces the solution of the master equation in the ensemble average [21]. In order to calculate the ensemble average of the above defined quantum trajectories, I consider the projector $\hat{\mathsf{P}} = |\psi\rangle\langle\psi|$ and its differential increment,

$$\begin{aligned} \mathrm{d}\hat{\mathsf{P}} &= |\psi + \mathrm{d}\psi\rangle\langle\psi + \mathrm{d}\psi| - |\psi\rangle\langle\psi| \\ &= |\mathrm{d}\psi\rangle\langle\psi| + |\psi\rangle\langle\mathrm{d}\psi| + |\mathrm{d}\psi\rangle\langle\mathrm{d}\psi|. \end{aligned} \tag{3.105}$$

Notice that the third summand with the two differentials could be neglected if the quantum trajectory was deterministic, since it would produce a term of the order $(\mathrm{d}t)^2$. However, as we have already seen in the previous chapter, for stochastic trajectories one needs to take into account higher order terms. The time derivative of the ensemble average of $\hat{\mathsf{P}}$ is now readily obtained,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}\left[\hat{\mathsf{P}}\right] \equiv \frac{\mathrm{E}\left[\mathrm{d}\hat{\mathsf{P}}\right]}{\mathrm{d}t} = \frac{1}{\mathrm{d}t}\mathrm{E}\left[|\mathrm{d}\psi\rangle\langle\psi| + |\psi\rangle\langle\mathrm{d}\psi| + |\mathrm{d}\psi\rangle\langle\mathrm{d}\psi|\right]. \tag{3.106}$$

By using the pointer state unraveling (3.101), the first and second summand of Eq. (3.106) read

$$\mathrm{E}\left[\hat{\mathsf{N}}\left[\psi\right]\hat{\mathsf{P}} + \hat{\mathsf{P}}\hat{\mathsf{N}}^{\dagger}\left[\psi\right] + \sum_i \left(\frac{\hat{\mathsf{J}}_i\left[\psi\right]}{\sqrt{r_i}} - 1\right) r_i \hat{\mathsf{P}} + \hat{\mathsf{P}} \sum_i \left(\frac{\hat{\mathsf{J}}_i^{\dagger}\left[\psi\right]}{\sqrt{r_i}} - 1\right) r_i\right]. \tag{3.107}$$

For the evaluation of the third and fourth summand of the above equation, one uses that the state $|\psi\rangle$ is non-anticipating[3], which renders the prefactors of the Poisson increments $\mathrm{d}N_i(t)$ in the unraveling (3.101) non-anticipating. Therefore, the ensemble averages can be factorized:

$$\mathrm{E}\left[f_i\left[\psi\right]\mathrm{d}N_i(t)\right] = \mathrm{E}\left[f_i\left[\psi\right]\right]\mathrm{E}\left[\mathrm{d}N_i(t)\right] = \mathrm{E}\left[f_i\left[\psi\right]\right] r_i \mathrm{d}t = \mathrm{E}\left[f_i\left[\psi\right] r_i\right]\mathrm{d}t, \tag{3.108}$$

with the jump rate r_i defined in Eq.(3.103).

The third summand of Eq. (3.106) is evaluated accordingly and gives

$$\begin{aligned} \mathrm{E}\left[\sum_i \left(\frac{\hat{\mathsf{J}}_i\left[\psi\right]}{\sqrt{r_i}} - 1\right)\hat{\mathsf{P}}\left(\frac{\hat{\mathsf{J}}_i^{\dagger}\left[\psi\right]}{\sqrt{r_i}} - 1\right) r_i\right] &= \mathrm{E}\left[\sum_i \left(\hat{\mathsf{J}}_i\left[\psi\right]\hat{\mathsf{P}}\hat{\mathsf{J}}_i^{\dagger}\left[\psi\right] - r_i\hat{\mathsf{P}}\right)\right] \\ &\quad - \mathrm{E}\left[\sum_i \left(\frac{\hat{\mathsf{J}}_i\left[\psi\right]}{\sqrt{r_i}} - 1\right) r_i\hat{\mathsf{P}} + \hat{\mathsf{P}}\sum_i \left(\frac{\hat{\mathsf{J}}_i^{\dagger}\left[\psi\right]}{\sqrt{r_i}} - 1\right) r_i\right], \end{aligned} \tag{3.109}$$

[3] A non-anticipating function was already introduced in Chapter 2 for classical stochastic processes. It requires that the function does only depend on times $s \leq t$ if the Poisson increment is evaluated at t.

where the Poisson rule (2.90) is used. By inserting Eqs. (3.107) and (3.109) into Eq. (3.106) and by using the explicit representations of the nonlinear operators $\hat{\mathsf{N}}[\psi]$ and $\hat{\mathsf{J}}[\psi]$ from Eqs. (3.96) and (3.102), one gets

$$\frac{\mathrm{E}\left[\mathrm{d}\hat{\mathsf{P}}\right]}{\mathrm{d}t} = \mathrm{E}\left[\frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}},\hat{\mathsf{P}}\right] + \sum_i \left(\overline{L_i^\dagger L_i}\hat{\mathsf{P}} - \frac{1}{2}\left\{\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i,\hat{\mathsf{P}}\right\} + \overline{L_i^\dagger}\hat{\mathsf{L}}_i\hat{\mathsf{P}} + \hat{\mathsf{P}}\hat{\mathsf{L}}_i^\dagger\overline{L}_i - 2\overline{L_i^\dagger}\overline{L}_i\hat{\mathsf{P}}\right)\right] + \mathrm{E}\left[\sum_i\left(\hat{\mathsf{L}}_i\hat{\mathsf{P}}\hat{\mathsf{L}}_i^\dagger + \overline{L_i^\dagger}\overline{L}_i\hat{\mathsf{P}} - \hat{\mathsf{L}}_i\hat{\mathsf{P}}\overline{L_i^\dagger} - \overline{L}_i\hat{\mathsf{P}}\hat{\mathsf{L}}_i^\dagger - r_i\hat{\mathsf{P}}\right)\right]. \quad (3.110)$$

One readily checks that all terms including ensemble averages of the Lindblad operators sum up to zero; in this context, Eq. (3.103) for the jump rates r_i has to be used. Finally, one uses that the ensemble average affects only ψ-dependent terms, which excludes the operators, specifically, the Hamiltonian $\hat{\mathsf{H}}$ and the Lindblad operators $\hat{\mathsf{L}}_i$. This leads to the Lindblad master equation (3.39)

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}},\rho\right] + \sum_i\left(\hat{\mathsf{L}}_i\rho\hat{\mathsf{L}}_i^\dagger - \frac{1}{2}\left\{\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i,\rho\right\}\right), \quad (3.111)$$

where the ensemble average of the projector equals the density matrix of the system, $\mathrm{E}\left[\hat{\mathsf{P}}\right] = \rho$.

3.7.3. Jump rate

The *total jump rate* of the unraveling is defined by the sum over the rates of all jumps,

$$r = \sum_i r_i. \quad (3.112)$$

Interestingly, one shows by a simple calculation that r is proportional to the linear entropy production (3.95) of the state $|\psi\rangle$. As in the previous section, one uses the projector $\hat{\mathsf{P}} = |\psi\rangle\langle\psi|$ to calculate

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}S_{\mathrm{lin}}\left[\hat{\mathsf{P}}\right] &= -2\mathrm{Tr}\left[\hat{\mathsf{P}}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathsf{P}}\right] \\ &= -2\langle\psi|\left[\frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}},\hat{\mathsf{P}}\right] + \sum_i\left(\hat{\mathsf{L}}_i\hat{\mathsf{P}}\hat{\mathsf{L}}_i^\dagger - \frac{1}{2}\left\{\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i,\hat{\mathsf{P}}\right\}\right)\right]|\psi\rangle \\ &= 2r, \end{aligned} \quad (3.113)$$

where it is used that $\hat{\mathsf{P}}$ evolves according to the Lindblad master equation (3.39).

Pointer states of the damped harmonic oscillator In Section 3.6.2, I presented two candidates for the pointer states of the damped harmonic oscillator: the coherent states and the Fock states. According to the predictability sieve, it was argued that due

to the fact that the former have a vanishing linear entropy production rate while the latter do not, only the coherent states are chosen as the pointer states. The pointer state unraveling together with Eq. (3.113) for the total jump rate, now allows one to interpret the solutions of the NLPSE without consulting the predictability sieve: The Fock states have a nonvanishing total jump rate r and therefore the quantum trajectory will be in such a state only for a relatively short time. In contrast to that, the coherent states have a vanishing jump rate such that the quantum trajectory stays in that state, once it has been reached by the NLPSE. Consequently, only the coherent states are the pointer states of the damped harmonic oscillator.

In general, one expects the pointer state unraveling to dynamically select the pointer states by the interplay of its deterministic and stochastic part. The deterministic NLPSE leads to candidate pointer states and the stochastic jump part ensures that those states, which have the lowest entropy production, survive the longest in the unraveling and correspond to the pointer states. This is in accordance with the predictability sieve criterion [19], which selects the states of lowest entropy production, i.e. with the lowest jump rate, as the pointer states. Additionally, in Ref. [70] it is shown that one can arrive at the pointer state unraveling by minimizing the jump rate of a piecewise deterministic unraveling, which implies that the pointer state unraveling has the minimal total jump rate and that the jump rate cannot sink below the linear entropy production rate.

4. Unraveling quantum Brownian motion

The master equation of quantum Brownian motion (QBM) was already introduced in Section 3.4. There, we examined its decoherence properties and deduced the equations of motion for the first and second moments of the phase space coordinates. In this chapter, I present the pointer states of QBM and perform an unraveling of the master equation, which yields the pointer states moving on phase space trajectories. In the semiclassical limit, one discovers the stochastic equation of motion for the pointer states as expected by classical Brownian motion (CBM) [71].

4.1. Pointer states

4.1.1. Solution of the NLPSE

The pointer states of QBM are obtained with the help of the NLPSE introduced in Eq. (3.96) of Section 3.6.1. The Hamiltonian and the Lindblad operator are taken from Eqs. (3.62), where the master equation is introduced in its dimensionless form. For the NLPSE, one obtains

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{\mathsf{N}}[\psi]|\psi\rangle = \Bigg\{ &-\mathrm{i}\frac{\kappa}{2}\left(\hat{\mathsf{p}}^2 - \overline{p^2}\right) + \kappa^2\left(V_x - (\hat{\mathsf{x}} - \overline{x})^2\right) + \frac{1}{16}\left(V_p - (\hat{\mathsf{p}} - \overline{p})^2\right) \\ &+ \frac{\kappa}{4}\left(\mathrm{i}C_{xp} - \frac{1}{\kappa}\right) - \mathrm{i}\frac{\kappa}{2}\left(\hat{\mathsf{x}} - \overline{x}\right)\left(\hat{\mathsf{p}} + \overline{p}\right)\Bigg\}|\psi\rangle. \end{aligned} \tag{4.1}$$

Note that due to the time dependence of the state $|\psi\rangle$ all expectation values are time-dependent, as well.

For the solution of the NLPSE, I make the Gaussian ansatz

$$\psi(x) = \frac{1}{(2\pi V_x)^{1/4}} \exp\left(-\frac{(x-\overline{x})^2}{4V_x}\left(1 - \mathrm{i}\kappa C_{xp}\right) + \mathrm{i}\kappa\left(x - \overline{x}\right)\overline{p} + \mathrm{i}\phi\right), \tag{4.2}$$

where ϕ is a time-dependent global phase. It is similar to the solution of the free Schrödinger equation presented in Section 3.1.3 and the confirmation that it provides a solution goes along the same line. The time derivative as well as the first and second spatial derivatives of $\psi(x)$ are readily obtained from Eqs. (3.15) and they are inserted into the NLPSE. Then, a comparison of coefficients in powers of $x - \overline{x}$ yields a closed

set of differential equations for the first moments and the variances,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\overline{x} &= \overline{p}, \\
\frac{\mathrm{d}}{\mathrm{d}t}\overline{p} &= -\overline{p}, \\
\frac{\mathrm{d}}{\mathrm{d}t}V_x &= C_{xp} - V_x\left(4\kappa^2 V_x - 1\right) + \frac{1-\kappa^2 C_{xp}^2}{16\kappa^2}, \\
\frac{\mathrm{d}}{\mathrm{d}t}C_{xp} &= \frac{1+\kappa^2 C_{xp}^2}{16\kappa^2}\,\frac{8-C_{xp}}{V_x} - 4\kappa^2 C_{xp} V_x.
\end{aligned} \tag{4.3}$$

Since $\psi(x)$ is a Gaussian, one can readily derive a differential equation for the momentum variance V_p from Eqs. (4.3) via the variance relation (3.14). Note that in the dimensionless units, defined in Eqs. (3.61), Eq. (3.14) takes the form

$$4V_x V_p = \frac{1}{\kappa^2} + C_{xp}^2. \tag{4.4}$$

In Eqs. (4.3), the differential equations for the first moments describe an exponential momentum damping, which reflects the friction experienced by the Brownian particle through the interaction with the gas environment. They have the same form as the corresponding equations of motion derived from the QBM master equation, cf. Eqs. (3.75) and (3.76). Notice that this movement does not affect the form of the wave packet but only its position in phase space. The last two equations in Eqs. (4.3), which describe the evolution of the variances, are much more complicated than those derived from the QBM master equation, see Eqs. (3.80). However, these two nonlinear differential equations exhibit stable fixed points, which can be evaluated analytically. They are obtained by solving the equations that arise by setting $\mathrm{d}V_x/\mathrm{d}t = \mathrm{d}C_{xp}/\mathrm{d}t = 0$ and read

$$\begin{aligned}
V_{x,\mathrm{ps}} &= \frac{1+\sqrt{1+\left(64\kappa^2+1\right)\sqrt{16\kappa^2+1}}}{8\kappa^2\sqrt{16\kappa^2+1}}, \\
C_{xp,\mathrm{ps}} &= \frac{4\kappa-\sqrt{\sqrt{16\kappa^2+1}-1}}{\kappa\sqrt{16\kappa^2+1}}.
\end{aligned} \tag{4.5}$$

$V_{p,\mathrm{ps}}$ can be calculated with the help of Eq. (4.4) and the label "ps" is an abbreviation of pointer state. The stability of the fixed points is confirmed by a linear stability analysis (see Appendix C.1).

A Gaussian wave packet (4.2) with the fixed variances (4.5) is a soliton-like solution in the sense that the form of the wave function in phase space does not change under the time evolution due to the NLPSE (4.1). Moreover, a numerical implementation of the NLPSE shows that this soliton-like solution is stable in the sense that any initial state turns into the above Gaussian. Therefore, this state is called a *pointer state of QBM* and I denote it by $|\pi(\overline{x},\overline{p})\rangle$, where $\overline{x}$ and $\overline{p}$ are its mean position and momentum coordinates. As Gaussian wave functions, the pointer states form an overcomplete basis

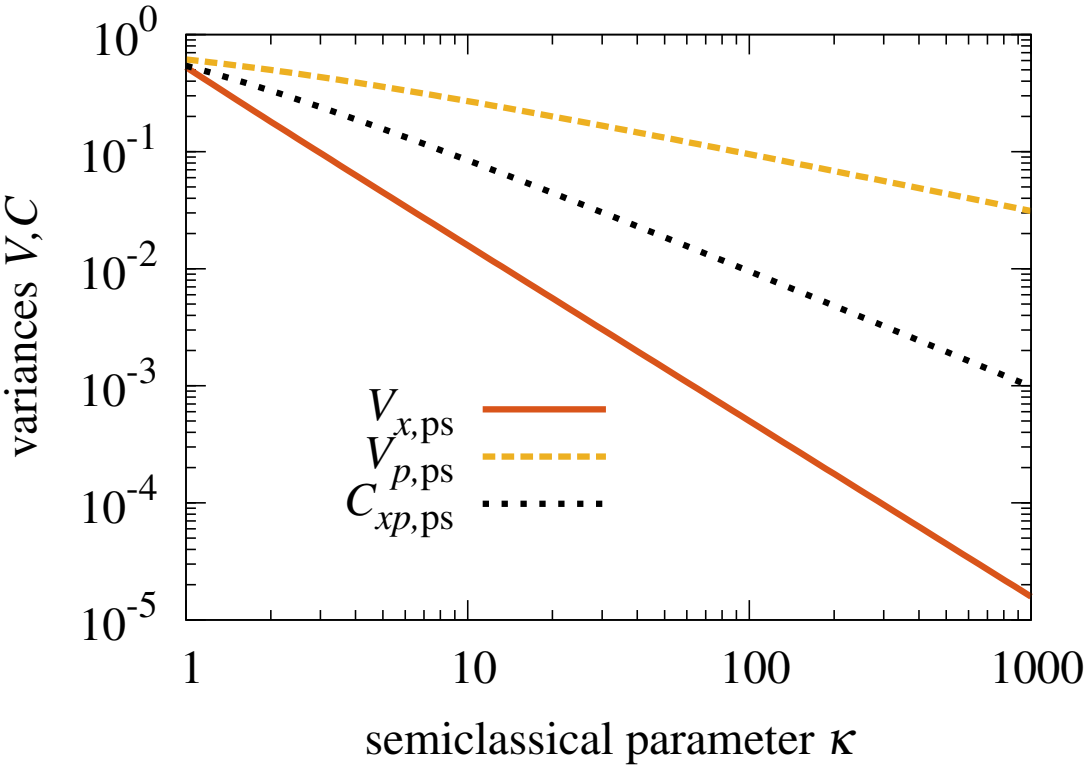

Figure 4.1.: Pointer state variances $V_{x,\mathrm{ps}}$ and $V_{p,\mathrm{ps}}$ in position (solid line) and momentum space (dashed line) and covariance $C_{xp,\mathrm{ps}}$ (dotted line) as a function of the semiclassical parameter κ. In the semiclassical regime ($\kappa \gg 1$), all curves follow a potential law.

set in Hilbert space and from Eqs. (4.5) one deduces their asymptotic widths as $\kappa \to \infty$,

$$\begin{aligned} V_{x,\mathrm{ps}} &\sim \frac{1}{2\kappa^{3/2}}, \\ V_{p,\mathrm{ps}} &\sim \frac{1}{\kappa^{1/2}}, \\ C_{xp,\mathrm{ps}} &\sim \frac{1}{\kappa}. \end{aligned} \tag{4.6}$$

The pointer states thus get more and more localized in phase space as one goes deeper into the semiclassical regime ($\hbar \to 0$) characterized by $\kappa \to \infty$, see Eq. (3.64). Figure 4.1 illustrates this point. Note that similar Gaussian states are obtained for pure spatial decoherence with $\hat{\mathsf{L}} = \hat{\mathsf{x}}$ [18, 63, 72] and for the damped harmonic oscillator, see Section 3.3. However, in difference to the aforementioned Gaussians, the covariance C_{xp} of the QBM pointer states is finite and depends on κ.

Extension to more dimensions Analogously to the discussion of the QBM master equation in Section 3.4.2, one obtains solutions of the NLPSE in more than one dimension as a product state of the one-dimensional pointer states (4.2).

4.1.2. Superposition of wave packets

Now, I consider the dynamics of a superposition state that consists of separated wave packets. It turns out that these superpositions are suppressed by the NLPSE until only a single localized state remains, which eventually turns into a pointer state $|\pi(\overline{x},\overline{p})\rangle$. This will lead to an understanding of how Born's rule arises in the course of the pointer state unraveling.

I consider an initial superposition state of the form

$$|\psi\rangle = \sum_{j=1}^{N} c_j(0)|\psi_j\rangle, \tag{4.7}$$

where the N wave packets $|\psi_j\rangle$ are well separated in phase space, orthogonal, and normalized. Each $|\psi_j\rangle$ has a weight

$$w_j(0) = |c_j(0)|^2, \tag{4.8}$$

with the $w_j(0)$ summing up to unity. Here and in the following, the time argument of the weights and amplitudes is dropped for better readability, and expectation values of the wave packet components are denoted as $\overline{A}_j = \langle\psi_j|\hat{\mathsf{A}}|\psi_j\rangle$; the variances and covariance are defined accordingly.

The $|\psi_j\rangle$ are required to be well separated wave packets in the sense that the overlap condition

$$\langle\psi_j|\hat{\mathsf{A}}|\psi_k\rangle = \delta_{jk}\langle\psi_j|\hat{\mathsf{A}}|\psi_j\rangle \;\forall j,k, \tag{4.9}$$

holds for the operators $\hat{\mathsf{A}} \in \{\mathbb{1}, \hat{\mathsf{x}}, \hat{\mathsf{x}}^2, \hat{\mathsf{p}}, \hat{\mathsf{p}}^2, \hat{\mathsf{x}}\hat{\mathsf{p}} + \hat{\mathsf{p}}\hat{\mathsf{x}}\}$. The shape of the $|\psi_j\rangle$ can be arbitrary, but their widths in phase space shall be close to that of a pointer state. In particular, one has to require that the variances $V_{x,j}$ and $V_{p,j}$ of the wave packet components $|\psi_j\rangle$ exhibit the same dependence (4.6) on κ as the pointer state variances. Condition (4.9) can then be fulfilled arbitrarily well by increasing the parameter κ, which decreases the pointer state width in phase space according to (4.6), and thus further orthogonalizes the $|\psi_j\rangle$. The situation just described allows one to assume that the separation of the wave packets in phase space is much greater than their widths and one may write

$$\begin{aligned} (\overline{x}_j - \overline{x}_k)^2 &\gg V_{x,j} \text{ and } V_{x,k}, \\ (\overline{p}_j - \overline{p}_k)^2 &\gg V_{p,j} \text{ and } V_{p,k}, \end{aligned} \tag{4.10}$$

for $j \neq k$.

For the following, it is useful to express the expectation values of the superposition state $|\psi\rangle$ with the help of those of the constituting wave packets $|\psi_j\rangle$:

$$\begin{aligned}
\overline{x} &= \sum_{j=1}^{N} w_j \overline{x}_j, \\
\overline{p} &= \sum_{j=1}^{N} w_j \overline{p}_j, \\
V_x &= \sum_{j=1}^{N} w_j V_{x,j} + \frac{1}{2} \sum_{j,k=1}^{N} w_j w_k \left(\overline{x}_j - \overline{x}_k\right)^2, \\
V_p &= \sum_{j=1}^{N} w_j V_{p,j} + \frac{1}{2} \sum_{j,k=1}^{N} w_j w_k \left(\overline{p}_j - \overline{p}_k\right)^2, \\
C_{xp} &= \sum_{j=1}^{N} w_j C_{xp,j} + \sum_{j,k=1}^{N} w_j w_k \left(\overline{x}_j - \overline{x}_k\right)\left(\overline{p}_j - \overline{p}_k\right).
\end{aligned} \tag{4.11}$$

By inserting the superposition state (4.7) into the NLPSE (4.1), the latter can be rewritten as the sum

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \sum_{j=1}^{N} \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(c_j\right)|\psi_j\rangle + c_j \frac{\mathrm{d}}{\mathrm{d}t}|\psi_j\rangle \right) = \sum_{j=1}^{N} c_j \hat{\mathsf{N}}[\psi]|\psi_j\rangle, \tag{4.12}$$

where the nonlinear operator on the right-hand side contains expectation values with respect to $|\psi\rangle$. From this equation, I deduce a set of coupled equations for the *normalized* constituting wave packets $|\psi_j\rangle$ and their weights $w_j = |c_j|^2$ by inserting the expectation values (4.11) into the NLPSE (4.12):

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}|\psi_j\rangle &= \hat{\mathsf{N}}[\psi_j]|\psi_j\rangle + \left(\kappa\left(\hat{\mathsf{x}} - \overline{x}_j\right) + \frac{\mathrm{i}}{4}\left(\hat{\mathsf{p}} - \overline{p}_j\right)\right)\left(\kappa\left(\overline{x} - \overline{x}_j\right) - \frac{\mathrm{i}}{4}\left(\overline{p} - \overline{p}_j\right)\right)|\psi_j\rangle, \\
\frac{\mathrm{d}}{\mathrm{d}t}w_j &= w_j\left[2\kappa^2\left(V_x - V_{x,j} - \left(\overline{x} - \overline{x}_j\right)^2\right) + \frac{1}{8}\left(V_p - V_{p,j} - \left(\overline{p} - \overline{p}_j\right)^2\right)\right].
\end{aligned} \tag{4.13}$$

Notice that the nonlinear operator appearing in the first equation of (4.13) now only contains expectation values with respect to $|\psi_j\rangle$. Thus, the temporal evolution of the superposition state is decomposed into an equation of motion for each weight plus an evolution of each constituting wave packet. Of course, in general, these equations cannot be solved separately as they are coupled, for instance, through the appearance of the expectation values $\overline{x}$ and $\overline{p}$ and the variances V_x and V_p of the whole superposition state.

If there is only one constituent in the "superposition", Eqs. (4.13) turn consistently into the NLPSE (4.1) and the trivial evolution $\mathrm{d}w_j/\mathrm{d}t = 0$ for the weight. This is seen most clearly by looking at the differences of the expectation values, which vanish in that case. In case of a superposition of many separated wave packets, the dynamics of

each constituent $|\psi_j\rangle$ is for one thing governed by the NLPSE, which turns the wave packet into the pointer state. For another thing, there is the second summand in the first equation of (4.13) that couples the dynamics of all wave packets as well as of the weights and cannot be assessed that simply.

The coupled weight equations from Eqs. (4.13) exhibit a fixed point if a single w_j is equal to one, while all others are zero. It is checked by a linear stability analysis in Appendix C.2 that this fixed point is a stable one. Thus, the NLPSE suppresses superpositions of the form (4.7) since the dynamics of the weights always ends up in the stable fixed point. The associated single localized wave packet, say $|\psi_j\rangle$, then asymptotically turns into the pointer state $|\pi\left(\overline{x}_j, \overline{p}_j\right)\rangle$.

Superposition of two pointer states As an example, let us consider the suppression of a superposition state consisting of only two pointer states. For the first component $|\psi_1\rangle$ and its accompanied weight w_1, Eqs. (4.13) simplify to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}|\psi_1\rangle &= \hat{\mathsf{N}}[\psi_1]|\psi_1\rangle + w_2\lambda[\psi]\left(\kappa\left(\hat{\mathsf{x}}-\overline{x}_1\right)+\frac{\mathrm{i}}{4}\left(\hat{\mathsf{p}}-\overline{p}_1\right)\right)|\psi_j\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}w_1 &= 2\left|\lambda[\psi]\right|^2\left(2w_1-1\right)w_1w_2, \end{aligned} \tag{4.14}$$

with

$$\lambda[\psi] = \kappa\left(\overline{x}_2-\overline{x}_1\right)-\frac{\mathrm{i}}{4}\left(\overline{p}_2-\overline{p}_1\right). \tag{4.15}$$

From Eqs. (4.14), one sees that in the first equation the term additional to the NLPSE depends on the phase space distances $\overline{x}_2-\overline{x}_1$ and $\overline{p}_2-\overline{p}_1$ through $\lambda[\psi]$, while the weight equation depends on the corresponding squares. This justifies the assumption that the dynamics of the mean values $\overline{x}_{1,2}$ and $\overline{p}_{1,2}$ may be neglected on the timescale $1/2\left|\lambda[\psi]\right|^2$ on which the weights vary and the rate

$$\Lambda \equiv 2\left|\lambda\left[\psi\right]\right|^2 = 2\kappa^2\left(\overline{x}_2-\overline{x}_1\right)^2+\frac{1}{8}\left(\overline{p}_2-\overline{p}_1\right)^2, \tag{4.16}$$

becomes approximately independent of time. It is then possible to explicitly solve the weight equation in Eqs. (4.14),

$$w_1(t) = \frac{1}{2}\left(1+\frac{2w_1(0)-1}{\sqrt{1-4w_1(0)\left(1-w_1(0)\right)\left(1-\mathrm{e}^{-\Lambda t}\right)}}\right). \tag{4.17}$$

Depending on the initial value $w_1(0)$, the solution asymptotically tends to zero or one, see Fig. 4.2: w_1 gets larger if and only if it is already the greater of the two weights, otherwise it diminishes. Notice that this asymptotic behavior for the weights can already be infered from Eqs. (4.14) without having the solution (4.17) at hand.

If there exists a superposition of many wave packets, which, in addition, all have different widths, the situation becomes far more complex and cannot be captured intuitively. However, the eventual decay of the superposition into one of the components is certain, though it is not easily predictable, which component of the superposition will survive in the course of the evolution due to the weight equation in (4.13).

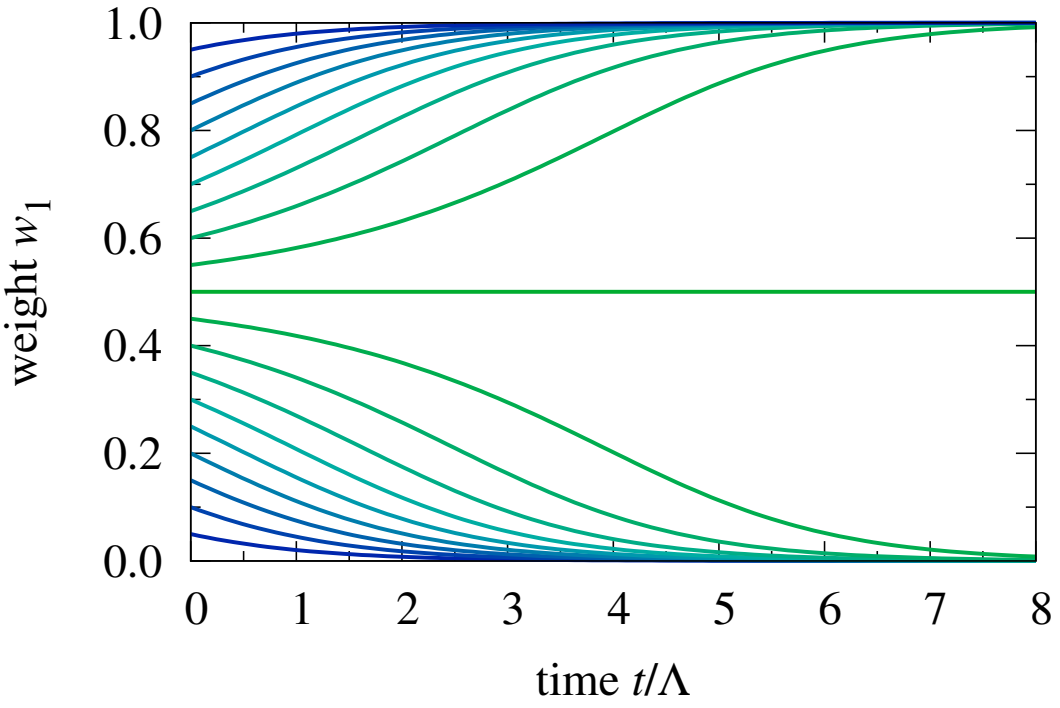

Figure 4.2.: Dynamics of the weight $w_1(t)$ of a superposition of two separated pointer states for different initial weights $w_1(0)$. If the initial weight is less than 0.5, it gets suppressed in the course of the evolution; if it is greater than 0.5, it tends to one. The time is plotted in units of the rate Λ.

4.2. Unraveling of the master equation

The dynamcis of the QBM master equation is now described by a particular ensemble of stochastic quantum trajectories, the pointer state unraveling. The NLPSE constitutes its deterministic part, which suppresses superpositions and leads to an asymptotic pointer state. However, since it is a deterministic equation, one would always obtain the same asymptotic state if starting in one particular superposition. In order for the evolution, to produce an ensemble of pointer states, which is in accordance with Born's rule (3.3), one needs to acount for the stochastic jump part of the unraveling. The stochastic part is also crucial for explaining the emergence of diffusive trajectories of the pointer state's location in phase space. Up to now, we know from the deterministic part that the pointer state trajectories undergo an exponential momentum damping. The stochastic motion of a *classical* Brownian particle is only obtained by incorporating the jump part as well.

According to Eq. (3.101), the pointer state unraveling has the form

$$|\mathrm{d}\psi\rangle = \hat{\mathsf{N}}\left[\psi\right]|\psi\rangle \mathrm{d}t + \left(\frac{\hat{\mathsf{J}}\left[\psi\right]}{\|\hat{\mathsf{J}}\left[\psi\right]|\psi\rangle\|} - 1\right)|\psi\rangle \mathrm{d}N, \tag{4.18}$$

with $\hat{\mathsf{N}}[\psi]$ the nonlinear operator of the NLPSE (4.1) and the single Poisson increment $\mathrm{d}N$. The nonlinear jump operator $\hat{\mathsf{J}}[\psi]$ is introduced in Eq. (3.102) and with the QBM Lindblad operator (3.62) it reads

$$\hat{\mathsf{J}}[\psi] = \sqrt{2}\left(\kappa\left(\hat{\mathsf{x}} - \overline{x}\right) + \frac{\mathrm{i}}{4}\left(\hat{\mathsf{p}} - \overline{p}\right)\right). \tag{4.19}$$

Finally, the jump rate of the Poisson process is obtained from Eq. (3.103),

$$r = \frac{\mathrm{E}\left[\mathrm{d}N\right]}{\mathrm{d}t} = \langle\psi|\hat{\mathsf{J}}^{\dagger}\left[\psi\right]\hat{\mathsf{J}}\left[\psi\right]|\psi\rangle = 2\kappa^2 V_x + \frac{1}{8}V_p - \frac{1}{2}. \tag{4.20}$$

4.2.1. Superposition states

Again, I consider the superposition (4.7) of separated wave packets $|\psi_j\rangle$, which fulfill the overlap relations (4.9) and whose widths in phase space are comparable to those of the pointer state. After a jump, this state reads

$$|\psi'\rangle = \frac{\hat{\mathsf{J}}[\psi]|\psi\rangle}{\sqrt{r}} = \sum_j c'_j|\psi'_j\rangle, \tag{4.21}$$

with the normalization factor determined by the jump rate r in Eq. (4.20). Furthermore, I introduce the normalized wave packets

$$|\psi'_j\rangle = \frac{\hat{\mathsf{J}}[\psi]|\psi_j\rangle}{\sqrt{\langle\hat{\mathsf{J}}^{\dagger}\hat{\mathsf{J}}\rangle_j}}, \tag{4.22}$$

involving the normalization factor

$$\langle \hat{\mathsf{J}}^\dagger \hat{\mathsf{J}} \rangle_j = \langle \psi_j | \hat{\mathsf{J}}^\dagger[\psi] \hat{\mathsf{J}}[\psi] | \psi_j \rangle = 2\kappa^2 \left(V_{x,j} + (\overline{x} - \overline{x}_j)^2 \right) + \frac{1}{8} \left(V_{p,j} + (\overline{p} - \overline{p}_j)^2 \right) - \frac{1}{2}. \tag{4.23}$$

Attention should be payed to the fact that the jump operator in (4.23) depends on the whole superposition state, whereas the expectation value is calculated with respect to $|\psi_j\rangle$. In the following, only the weights, i.e. the squared moduli $w'_j = \left| c'_j \right|^2$, of the new coefficients after a jump will be required, for which one gets

$$w'_j = w_j \frac{\langle \hat{\mathsf{J}}^\dagger \hat{\mathsf{J}} \rangle_j}{r}. \tag{4.24}$$

The new wave packet components $|\psi'_j\rangle$ can be safely assumed to be still separated and localized because the jump operator modifies the shape only linearly in $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$. This means that the superposition state (4.21) after the jump is again a superposition of separated wave packets, but with different weights. In short, the effect of a jump can be approximately accounted for by a reshuffling of a finite number of weights w_j in the superposition. I confirmed this numerically by an implementation of the unraveling (4.18), see Section 4.2.3 for details about the numerics.

One can now approximately describe the time evolution of the weights as a classical SDE whose deterministic part, resulting from the dynamics of the NLPSE, is defined by the second equation of (4.13) and its stochastic part is characterized by Eq. (4.24):

$$\mathrm{d}w_j = w_j \left(r - \langle \hat{\mathsf{J}}^\dagger \hat{\mathsf{J}} \rangle_j \right) \mathrm{d}t + w_j \left(\frac{\langle \hat{\mathsf{J}}^\dagger \hat{\mathsf{J}} \rangle_j}{r} - 1 \right) \mathrm{d}N. \tag{4.25}$$

Here, the deterministic evolution of the weights from Eqs. (4.13) is rewritten into a more convenient form by using the jump rate r and the normalization factor $\langle \hat{\mathsf{J}}^\dagger \hat{\mathsf{J}} \rangle_j$ from Eqs. (4.20) and (4.23). By construction, the Poisson increment $\mathrm{d}N$ has the same statistical properties like that of the pointer state unraveling, which means that its ensemble average is $\mathrm{E}[\mathrm{d}N] = r\mathrm{d}t$.

Equation (4.25) describes the temporal evolution of the weights in a quantum trajectory. As one finds from the numerical simulation, the quantum trajectory of any initial superposition state of separated wave packets asymptotically turns into a pointer state and the stochastic motion of the weights ceases. The pointer state is characterized by a quantum trajectory where one of the weights equals one while all others vanish. In other words, exactly if the weight w_α approaches unity in the course of the evolution of the SDE (4.25), the asymptotic pointer state of the trajectory emerges from the component $|\psi_\alpha\rangle$ of the superposition and becomes $|\pi(\overline{x}_\alpha, \overline{p}_\alpha)\rangle$. Consequently, w_α vanishes in all cases where the pointer state emerges from a different component $|\psi_k\rangle$ with $k \neq \alpha$. Following this reasoning, the average value of $w_\alpha(t)$ for $t \to \infty$ equals the relative frequency of the pointer state $|\pi(\overline{x}_\alpha, \overline{p}_\alpha)\rangle$ in the ensemble of quantum trajectories.[1] That

[1] For clarity, I reintroduced the time argument of the weights.

is,

$$\mathrm{Prob}\left(\alpha|\psi\right) = \mathrm{E}\left[w_\alpha\left(t\to\infty\right)\right], \tag{4.26}$$

where $\mathrm{Prob}\left(\alpha|\psi\right)$ denotes the probability to end up in the pointer state $|\pi\left(\overline{x}_\alpha,\overline{p}_\alpha\right)\rangle$ provided the initial state is $|\psi\rangle$ from Eq. (4.7). From the SDE (4.25), one easily obtains

$$\mathrm{E}\left[\mathrm{d}w_\alpha(t)\right] = 0, \tag{4.27}$$

since the contributions from the deterministic and from the stochastic part cancel out. This implies that $\mathrm{E}\left[w_\alpha(t)\right] = \mathrm{const}$. In particular, for the initial weights $w_j(0) = |c_j(0)|^2$ one derives

$$\mathrm{E}\left[w_\alpha(t\to\infty)\right] = \mathrm{E}\left[w_\alpha(0)\right] = |c_\alpha(0)|^2. \tag{4.28}$$

As one directly sees from Eqs. (4.26) and (4.28), this confirmes the Born rule as written in Eq. (3.94) and shows that the pointer state unraveling produces the desired ensemble of pointer states.

Jump rates The jump rate of the unraveling differs significantly depending on the state of the quantum trajectory. In a superposition state (4.7) of separated wave packets, one gets for the jump rate by inserting Eqs. (4.11) into Eq. (4.20),

$$r = \sum_{j=1}^{N} w_j \left(2\kappa^2 V_{x,j} + \frac{1}{8}V_{p,j} - \frac{1}{2}\right) + \frac{1}{2}\sum_{j,k=1}^{N} w_j w_k \left(2\kappa^2\left(\overline{x}_j - \overline{x}_k\right)^2 + \frac{1}{8}\left(\overline{p}_j - \overline{p}_k\right)^2\right). \tag{4.29}$$

Since the phase space separation of the wave packets is assumed to be much greater than their widths, see Eq. (4.10), one deduces from the second term in Eq. (4.29) that the jump rate is much greater for a superposition state than for a single wave packet with variances in the vicinity of the pointer state variances. Thus, the trajectory experiences frequent jumps until the distribution of weights w_j has reduced all but a single component. The quantum trajectory then turns into a pointer state and stays in this state except for the weak stochastic perturbations described by the diminished jump rate as given by one summand of the first term in Eq. (4.29). This diminished jump rate causes the stochastic motion of the pointer state, which I investigate in the following.

4.2.2. Single wave packets

We have now understood how superposition states turn into a mixture of pointer states. It is the purpose of this section to explore how these localized states move around in phase space. In particular, I show how one can understand the emergence of a diffusive behavior of the pointer states, which leads to classical diffusion in the semiclassical limit.

In order to analyze the stochastic motion of a single wave packet in the unraveling, I consider a pointer state $|\pi\left(\overline{x},\overline{p}\right)\rangle$ that is moving on the deterministic phase space

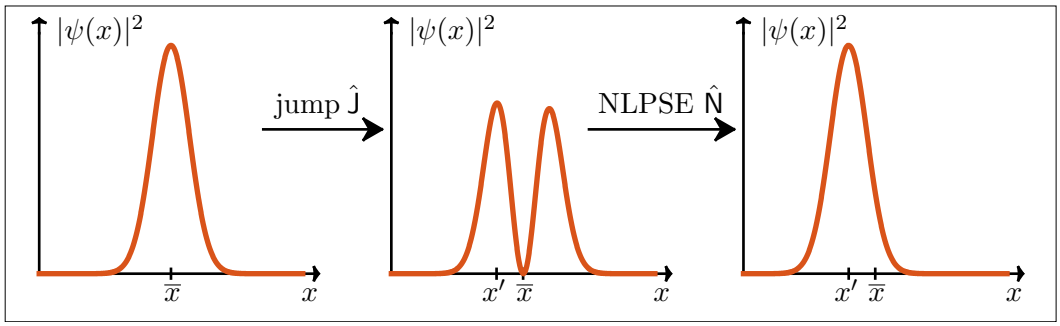

Figure 4.3.: Sketch of the simplified jump process: A jump turns the wave packet with mean position $\overline{x}$ into a slightly asymmetric double-peaked structure. The NLPSE then suppresses one of the peaks resulting in a single wave packet at the position $\overline{x}'$ of one of the double-peaks. A similar picture applies in momentum space.

trajectory as prescribed by the NLPSE (see Section 4.1.1). According to the unraveling (4.18)-(4.20), this motion is interrupted by jumps, which occur at a rate

$$r_{\mathrm{ps}} = 2\kappa^2 V_{x,\mathrm{ps}} + \frac{1}{8} V_{p,\mathrm{ps}} - \frac{1}{2}, \tag{4.30}$$

where the label "ps" denotes that it is a pointer state property, with the pointer state variances $V_{x,\mathrm{ps}}$ and $V_{p,\mathrm{ps}}$ defined via Eqs. (4.4) and (4.5). The normalized state after a jump is calculated by acting with the jump operator (4.19) on the pointer state (4.2). In position representation it reads

$$\langle x|\psi'\rangle = \frac{\langle x|\hat{\mathsf{J}}[\pi\,(\overline{x},\overline{p})]|\pi\,(\overline{x},\overline{p})\rangle}{\|\hat{\mathsf{J}}[\pi\,(\overline{x},\overline{p})]|\pi\,(\overline{x},\overline{p})\rangle\|} = \sqrt{\frac{2}{r_{\mathrm{ps}}}}\kappa \left(1 - \frac{1 - \mathrm{i}\kappa C_{xp,\mathrm{ps}}}{8\kappa^2 V_{x,\mathrm{ps}}}\right)(x - \overline{x})\,\langle x|\pi\,(\overline{x},\overline{p})\rangle, \tag{4.31}$$

which is a symmetric double-peaked structure that vanishes at $\overline{x}$. One gets a similar double-peaked structure for the momentum representation $\langle p|\psi'\rangle$. The symmetry in this state occurs because a symmetric state was assumed before the jump. However, in reality the system state is never exactly symmetric and a jump produces a double-peaked structure with slightly different peak heigths. Therefore, one deals with an *asymmetric* wave packet after a jump. From Eq. (4.17), prescribing the temporal evolution of the weights of a superposition of two wave packets, one sees that even small asymmetries in the peak heights are sufficient to suppress the lower peak, see also Fig. 4.2. As a consequence, the evolution of the NLPSE, which directly follows a jump, suppresses the double-peaked structure and leads to a re-emergence of a single wave packet, see Fig. 4.3. A simple analysis of the double-peaked structure in position and momentum space reveals that the subpeak at $\overline{p}' > \overline{p}$ "survives" if and only if the subpeak at $\overline{x}' > \overline{x}$ remains, where further details are given in Appendix C.3. This means that after a

jump and after the NLPSE has re-formed the pointer state, the position and momentum expectations are positively correlated.

It depends on the initial asymmetry, which of the two subpeaks of the double-peaked structure survives and turns into the single-peaked wave packet. Without further information, it is reasonable to assume an unbiased distribution of the asymmetry, which leads to equal probabilities for both subpeaks. In addition, I assume that the single-peaked state is restored sufficiently fast by the NLPSE, such that no jump interferes during this process. Further jumps occur only after a localized single wave packet has re-formed. As a result, together with the two assumptions, the process described above and sketched in Fig. 4.3, defines effectively a jump of the pointer state's first moments in phase space. The lengths of the phase space jump can be calculated easily from the positions of the two subpeaks of state (4.31) after the jump,

$$\begin{aligned} j_x &= \left|\overline{x}' - \overline{x}\right| = \sqrt{2V_{x,\mathrm{ps}}}, \\ j_p &= \left|\overline{p}' - \overline{p}\right| = \sqrt{2V_{p,\mathrm{ps}}}. \end{aligned} \tag{4.32}$$

Since the position and momentum expectation values are positively correlated, one arrives at the two possible jumps

$$\boldsymbol{j}_1 = \begin{pmatrix} j_x \\ j_p \end{pmatrix} \text{ and } \boldsymbol{j}_2 = \begin{pmatrix} -j_x \\ -j_p \end{pmatrix}. \tag{4.33}$$

As we have just seen, every jump of the pointer state unraveling (4.18) results in an effective phase space jump of the pointer state. The jumps occur at a rate r_{ps}, see Eq. (4.30), and because I assumed equal probability to go left or right, the rates r_1 and r_2 of the Poisson processes $\mathrm{d}N_1$ and $\mathrm{d}N_2$, characterizing the jumps (4.33), are given by

$$r_{1,2} = \frac{\mathrm{E}\left[\mathrm{d}N_{1,2}\right]}{\mathrm{d}t} = \frac{r_{\mathrm{ps}}}{2}. \tag{4.34}$$

This simple jump model puts one in the position to write down a SDE for $\overline{x}$ and $\overline{p}$,

$$\begin{pmatrix} \mathrm{d}\overline{x} \\ \mathrm{d}\overline{p} \end{pmatrix} = \begin{pmatrix} \overline{p} \\ -\overline{p} \end{pmatrix} \mathrm{d}t + \begin{pmatrix} j_x \\ j_p \end{pmatrix} \left(\mathrm{d}N_1 - \mathrm{d}N_2\right). \tag{4.35}$$

Here, the deterministic evolution is taken from Eqs. (4.3) in Section 4.1.1, and the stochastic jumps are composed of the two Poisson processes as described above. This SDE has a form similar to the random walk considered in Eq. (2.103) in Section 2.5.3. In particular, both the $\overline{x}$- and $\overline{p}$-components are random walks complemented by a drift. As usual for calculations with SDEs of the above kind, it is sufficient to consider terms to first order in $\mathrm{d}t$ only. Therefore, the drift term appears only in the first moments of $\mathrm{d}\overline{x}$ and $\mathrm{d}\overline{p}$, whereas all higher moments are determined solely by the jump part. Following the calculation of the moments of the random walk in Section 2.5.3, one obtains for the

moments of the SDE (4.35)

$$\begin{aligned} \mathrm{E}[\mathrm{d}\overline{x}] &= \overline{p}\mathrm{d}t, & \mathrm{E}[\mathrm{d}\overline{p}] &= -\overline{p}\mathrm{d}t, \\ \mathrm{E}[(\mathrm{d}\overline{x})^{2n}] &= j_x^{2n} r_{\mathrm{ps}}\mathrm{d}t, & \mathrm{E}[(\mathrm{d}\overline{p})^{2n}] &= j_p^{2n} r_{\mathrm{ps}}\mathrm{d}t, \\ \mathrm{E}[(\mathrm{d}\overline{x})^{2n+1}] &= 0, & \mathrm{E}[(\mathrm{d}\overline{p})^{2n+1}] &= 0, \\ \mathrm{E}[(\mathrm{d}\overline{x}\mathrm{d}\overline{p})^{n}] &= (j_x j_p)^n \, r_{\mathrm{ps}}\mathrm{d}t, \end{aligned} \tag{4.36}$$

for $n \geq 1$.

The dependence of the moments (4.36) on κ in the semiclassical limit, $\kappa \to \infty$, can now be infered by using the jump rate (4.30), the jump widths (4.32), and the asymptotic pointer state's widths (4.6). It is readily seen that the rate of jumps increases, whereas their widths decrease as one goes further into the semiclassical regime. If CBM arises as the limit of QBM, the jump process should turn into a diffusion process, i.e. it must have a diffusive limit. To verify this, the three second-order moments of $\mathrm{d}\overline{x}$ and $\mathrm{d}\overline{p}$ are calculated as $\kappa \to \infty$:

$$\begin{aligned} \mathrm{E}[(\mathrm{d}\overline{x})^2] &= j_x^2 r_{\mathrm{ps}}\mathrm{d}t \sim \frac{1}{\kappa}\mathrm{d}t, \\ \mathrm{E}[(\mathrm{d}\overline{p})^2] &= j_p^2 r_{\mathrm{ps}}\mathrm{d}t \sim 2\mathrm{d}t, \\ \mathrm{E}[\mathrm{d}\overline{x}\mathrm{d}\overline{p}] &= j_x j_p r_{\mathrm{ps}}\mathrm{d}t \sim \sqrt{\frac{2}{\kappa}}\mathrm{d}t. \end{aligned} \tag{4.37}$$

Hence, the second moment of $\mathrm{d}\overline{p}$ is indeed finite in the semiclassical limit, which corresponds to the momentum diffusion exhibited in CBM. The other two second moments vanish as $\kappa \to \infty$.

It is now clear that, for describing the behavior of the phase space jumps for large κ, it is convenient and legitimate to approximate the SDE (4.35) by a diffusive SDE like that introduced as phase space diffusion (2.63) in Section 2.4. It follows that the diffusion constants of this phase space diffusion have to be identified with

$$\begin{aligned} D_x &= j_x^2 r_{\mathrm{ps}} \sim \frac{1}{\kappa}, \\ D_p &= j_p^2 r_{\mathrm{ps}} \sim 2, \\ D_{xp} &= j_x j_p r_{\mathrm{ps}} \sim \sqrt{\frac{2}{\kappa}}, \end{aligned} \tag{4.38}$$

as $\kappa \to \infty$. In the semiclassical limit, the phase space diffusion reduces to a momentum diffusion with $D_p = 2$ that we already recognized as CBM in Section 2.4.3. Written in physical units, which are defined via Eqs. (3.61), one finally arrives at the Langevin equation of CBM for the evolution of the mean momentum of the pointer state in phase space,

$$\mathrm{d}\overline{p} = -2\gamma\overline{p}\mathrm{d}t + \sqrt{4\gamma m k_{\mathrm{B}} T_{\mathrm{env}}}\mathrm{d}W, \tag{4.39}$$

where the Wiener increment $\mathrm{d}W$ has the dimension of a square root of time.

It should be remarked here, that the crucial assumption leading to this model is the *immediate* restoration of the pointer state after a jump. The real dynamics displayed by

the quantum trajectories will take a finite time until the double-peaked wave function returns to a pointer state, and there may be several jumps in between. I show in the following, by numerically simulating trajectories of the pointer state unraveling, that this is indeed the case giving rise to complex dynamics. Nonetheless, the general picture of the analytic model can be confirmed.

4.2.3. Numerical study of pointer state trajectories

I propagate the deterministic part of the pointer state unraveling (4.18) by using a combination of the Crank–Nicolson method and a split-operator technique [73–75]. The split-operator technique is an efficient method to solve equations of motion where the individual terms depend either on the position or on the momentum operator. However, for terms with a mixed operator dependence like $\hat{\mathsf{x}}\hat{\mathsf{p}}$ this does not work and they need to be propagated directly, for instance, with the help of the Crank–Nicolson method. The jump part is accounted for by a straightforward implementation of a Poisson process, which involves sampling from the accompanied waiting-time distribution. If a jump occurs, it is carried out according to Eq. (4.18).

In this way, I generated a sample of quantum trajectories and calculated their individual first moments $\overline{x}$ and $\overline{p}$ as well as their variances V_x, V_p, and C_{xp}. Figure 4.4 shows exemplarily the temporal evolution of $\overline{p}$ and V_p for two sample trajectories. One clearly observes the jump-like behavior of the trajectories as expected for a piecewise deterministic unraveling. Examination of Fig. 4.4(b) shows that a pointer state, characterized by its constant variance, turns into a different state upon a jump, which is evident from the increase of the variance of the state. Unlike the assumption of the analytic model of the previous section, there is, in general, a whole set of jumps before the pointer state is restored. A similar behavior is found in position space, which I do not show here.

Conclusions about a stochastic model that describes the first moments of the quantum trajectories can be drawn by examination of the temporal evolution of the *unbiased estimators* of a finite sample of N trajectories,

$$\begin{aligned}
m_N[x] &= \frac{1}{N}\sum_{i=1}^{N}\overline{x}_i, \\
m_N[p] &= \frac{1}{N}\sum_{i=1}^{N}\overline{p}_i, \\
s_N^2[x] &= \frac{1}{N-1}\sum_{i=1}^{N}\left(\overline{x}_i - m_N[x]\right)^2, \\
s_N^2[p] &= \frac{1}{N-1}\sum_{i=1}^{N}\left(\overline{p}_i - m_N[p]\right)^2, \\
c_N[x,p] &= \frac{1}{N-1}\sum_{i=1}^{N}\left(\overline{x}_i - m_N[x]\right)\left(\overline{p}_i - m_N[p]\right),
\end{aligned} \tag{4.40}$$

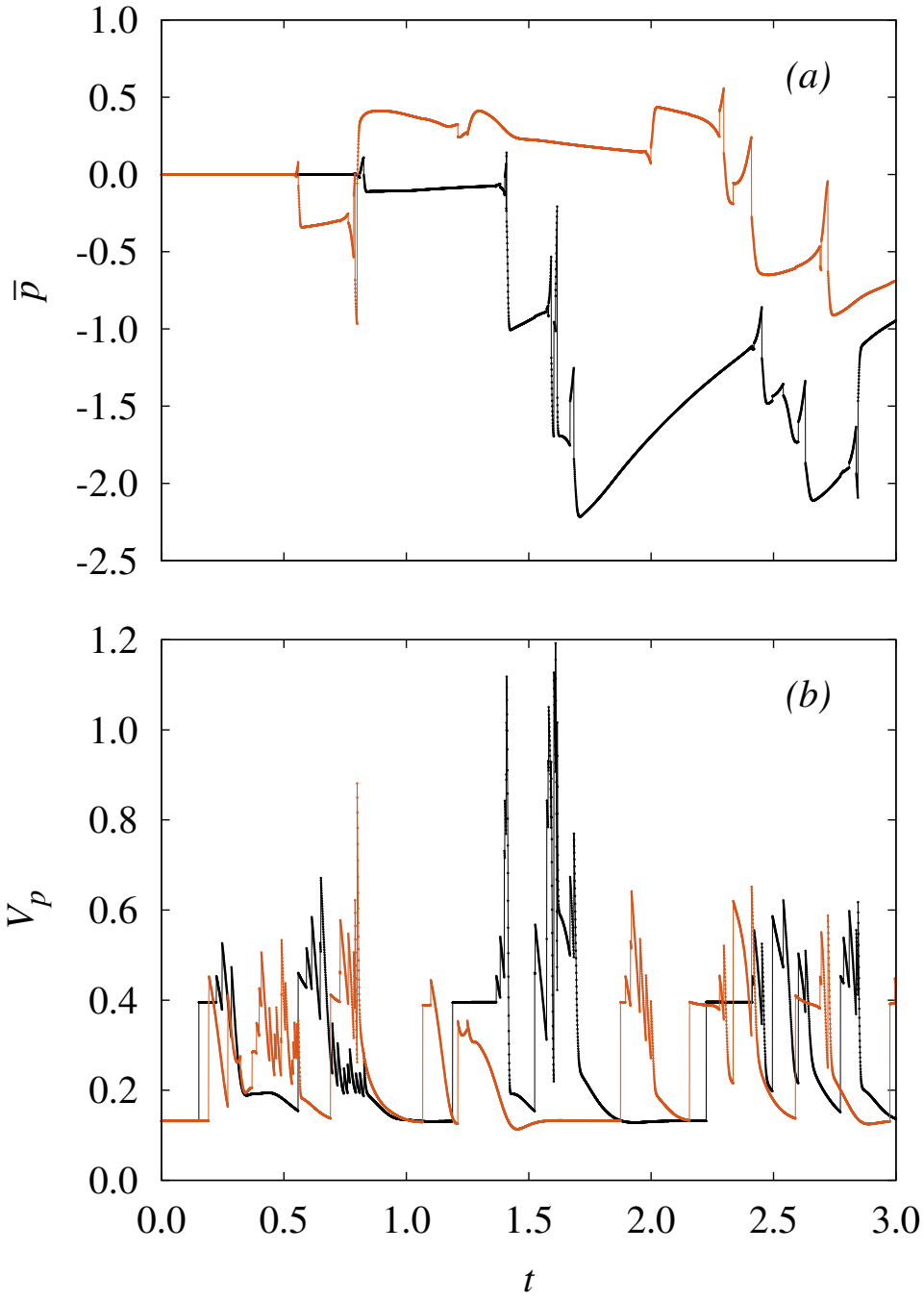

Figure 4.4.: (a) Mean momentum $\overline{p}$ and (b) momentum variance V_p of two sample quantum trajectories starting at the same pointer state $|\pi(0,0)\rangle$. From (b) one observes that, in general, more than a single jump occurs before the width of the wave function is restored to the pointer state width. The calculations are made at $\kappa = 50$.

where $\overline{x}_i$, $\overline{p}_i$ are the first moments of quantum trajectory i. With $m_N[\cdot]$, $s_N^2[\cdot]$, and $c_N[x,p]$ I denote the estimators for the phase space mean values, the corresponding variances, and the covariance. In Figs. 4.5 and 4.6, I show the sample estimators of the position and momentum variance as well as of the covariance. Both $s_N^2[p]$ and $c_N[x,p]$ asymptotically tend to a constant value, whereas $s_N^2[x]$ grows linearly with time for large times; a behavior that we already know from phase space diffusion, see Eqs. (2.71). Therefore, I describe $\overline{x}_i$, $\overline{p}_i$ by the SDE (2.63) of the phase space diffusion introduced in Section 2.4. Due to the finite sample size, all estimators are stochastic quantities. To estimate their standard deviations, I use the phase space diffusion model, which I show in Appendix A.1. For the variances and the covariance, they are shown as dotted lines in Figs. 4.5 and 4.6 and read

$$\begin{aligned}
\sigma_{s_N^2[x]} &= \sqrt{\frac{2}{N-1}}\mathrm{Var}[x], \\
\sigma_{s_N^2[p]} &= \sqrt{\frac{2}{N-1}}\mathrm{Var}[p], \\
\sigma_{c_N[x,p]} &= \sqrt{\frac{1}{N-1}}\sqrt{\mathrm{Var}\,[x]\,\mathrm{Var}\,[p] + \mathrm{Cov}\,[x,p]^2}.
\end{aligned} \tag{4.41}$$

As one can see in the figures, the fluctuations of the sample variances and the covariance are well described by Eqs. (4.41). The same holds for the estimators of the first moments $m_N[x]$ and $m_N[p]$, which I do not show here.

Extraction of the diffusion constants One extracts the diffusion constants D_x, D_p, and D_{xp}, which occur in the phase space diffusion and are defined in Eqs. (2.69), by fitting the time dependence of the variances, see Eqs. (2.71), to those of the numerically generated sample. Since $\mathrm{Var}[p]$ only depends on D_p, and $\mathrm{Cov}[x,p]$ only depends on D_p and D_{xp}, fitting is done consecutively by extracting D_p from $s_N^2[p]$, D_{xp} from $c_N[x,p]$, and finally D_x from $s_N^2[x]$. The results for different κ alongside their counterparts calculated from the simplified analytic jump model in Eq. (4.38), are shown in Fig. 4.7. One observes that the momentum diffusion D_p from Eqs. (4.38), which is obtained from the jump model (4.35), is in good quantitative agreement with the simulation. The deviation of the theoretically calculated diffusion constants D_x and D_{xp} from the simulated ones is due to the crude simplification made by the assumption that a jump in the unraveling corresponds to a phase space jump of the pointer state without further dynamics; Fig. 4.4 shows clearly that this is not the case.

For large κ, i.e. in the semiclassical regime, both the analytic model and the numerical simulation exhibit the classically expected behavior. Specifically, the position diffusion D_x and the covariance diffusion D_{xp} tend to zero, whereas the momentum diffusion D_p approaches the value 2.

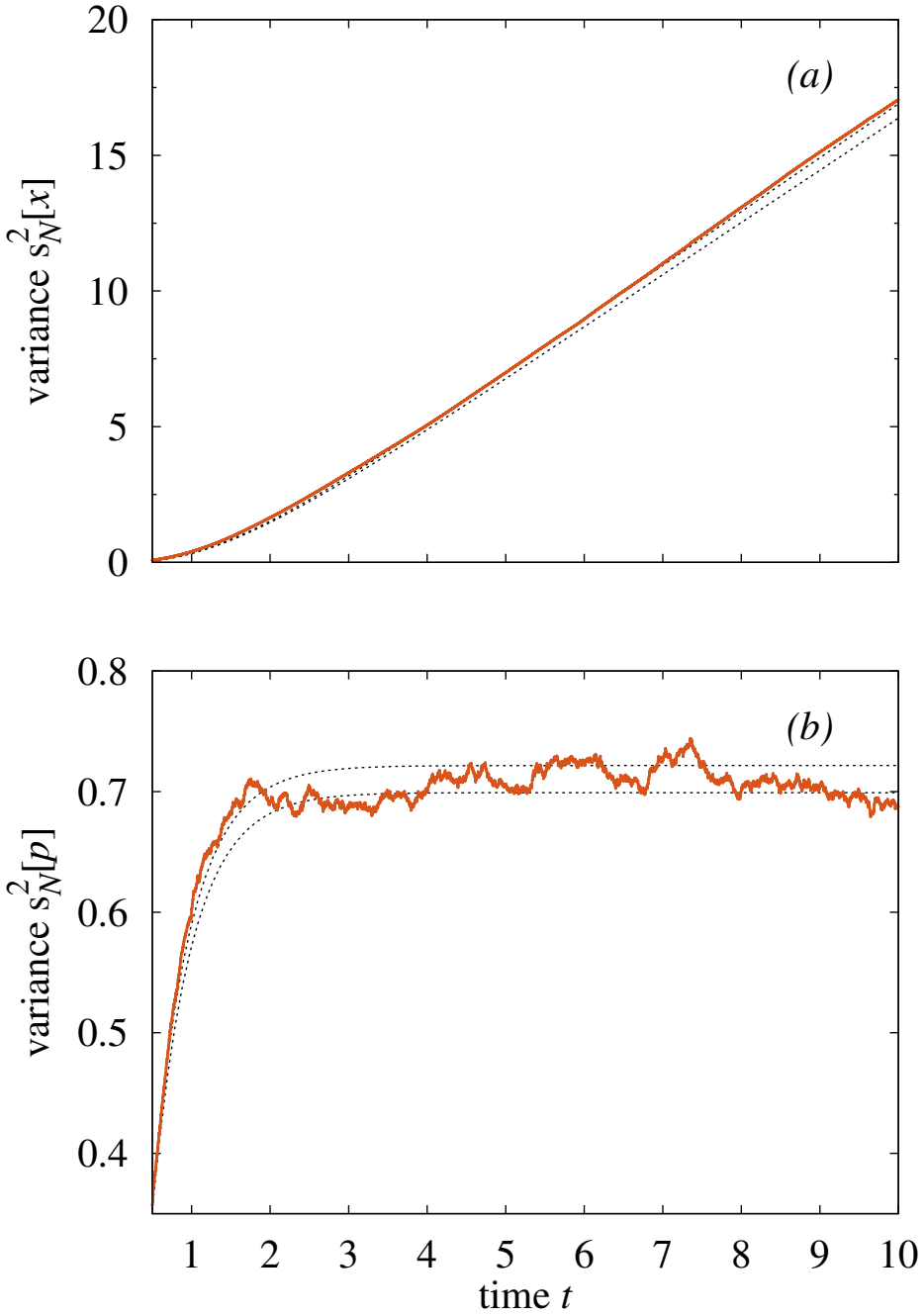

Figure 4.5.: (*a*) Position variance estimator $s_N^2[x]$ and (*b*) momentum variance estimator $s_N^2[p]$ of the numerically generated sample (solid) as well as their theoretically expected standard deviations $\mathrm{Var}[x] \pm \sigma_{s_N^2[x]}$ and $\mathrm{Var}[p] \pm \sigma_{s_N^2[p]}$ (dashed) according to the phase space diffusion model. The fluctuations are well characterized by the dashed lines. Calculations are done at $\kappa = 50$ for $N = 8000$ trajectories.

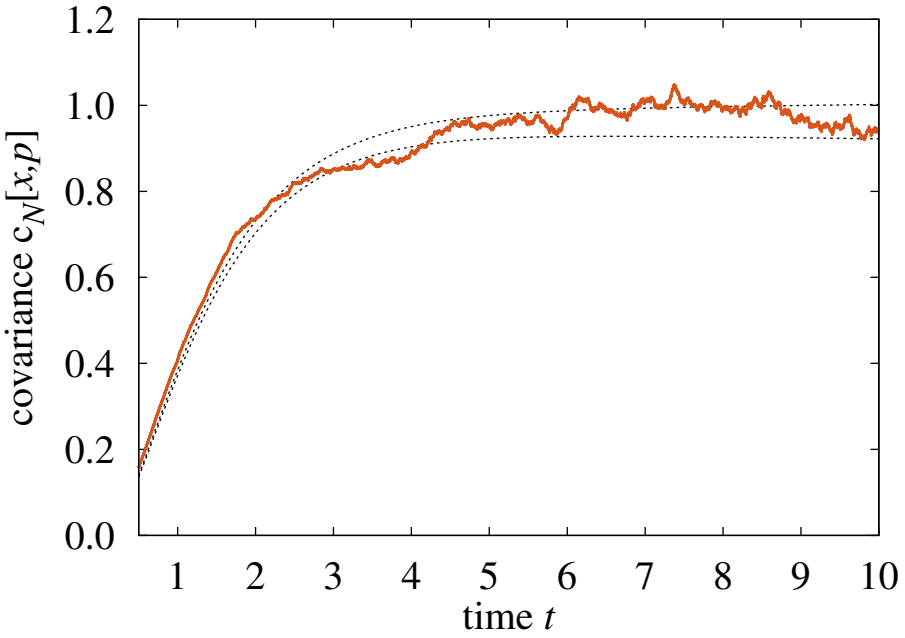

Figure 4.6.: Same as Fig. 4.5 for the estimator of the covariance $c_N[x,p]$.

4.3. Summary

By analyzing the pointer state unraveling of QBM, I have first shown that the pointer states are rotated Gaussians in phase space. Secondly, initial superpositions of separated wave packets evolve into a mixture of pointer states, a process that can be approximately described by a stochastic differential equation for the weights of the constituents. The probability of each pointer state in the mixture was shown to emerge according to Born's rule. If the state is a superposition of wave packets, the jump rate of the unraveling is much greater than for a single pointer-state-like wave packet. This diminished jump rate and a subtle interplay between the NLPSE and the stochastic jumps then lead to an effective random walk of the wave packet in phase space: The stochastic jump part of the quantum trajectory divides a wave packet into a double-peaked wave packet, which then returns to a pointer state at one of the positions of the double-peak. This restoration of the pointer state after a quantum jump is mediated by the deterministic part of the unraveling, the NLPSE. Effectively, this twofold process leads to a random walk of the pointer state's first moments in phase space. A conversion of this jump process into a phase space diffusion leads to the definition of the diffusion values in position and momentum as well as the covariance diffusion. In the semiclassical limit $\kappa \to \infty$, this diffusion process turns into the Langevin equation of CBM. Thus, starting from a purely quantum description of a dissipative system, I showed how a mixture of localized wave packets arises from a superposition, where each of constituent propagates along the classically expected trajectory in phase space. In this sense, one is able to understand the quantum-to-classical transition from QBM to CBM.

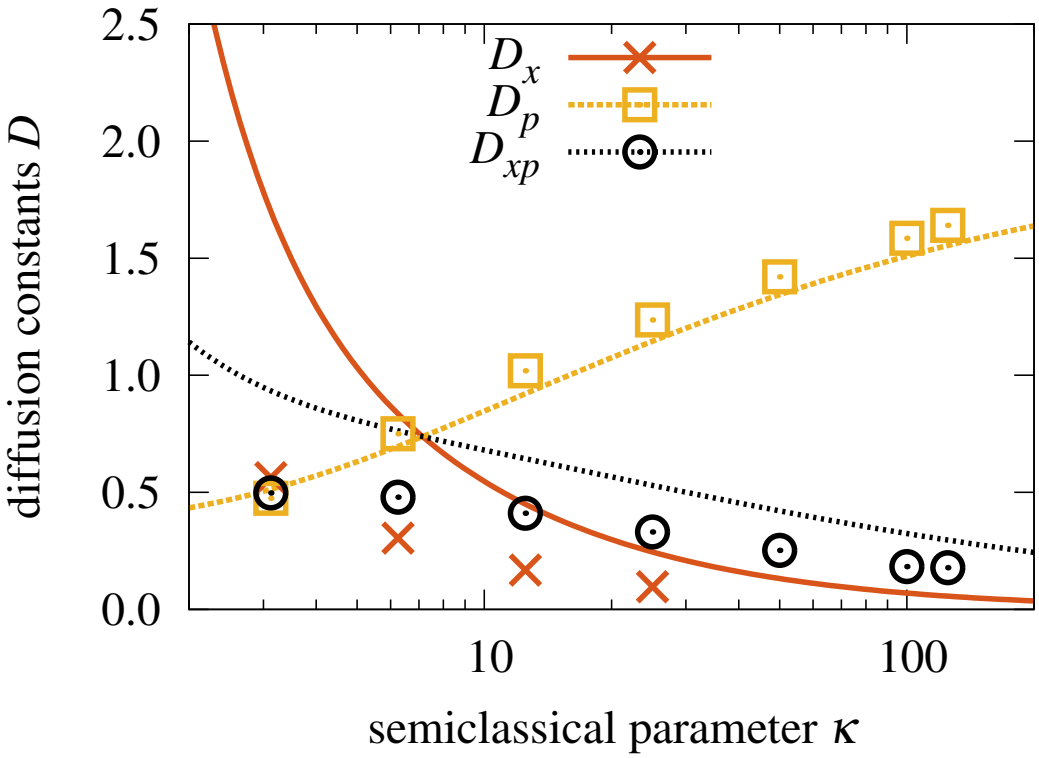

Figure 4.7.: Dependence of the diffusion constants D_x (solid line), D_p (dashed line) and D_{xp} (dotted line) on κ. The lines are calculated from Eqs. (4.38) of the analytic model, whereas the symbols represent the results of the numerical simulation. One observes for all three diffusion constants that the analytic model captures the main features of their dependence on κ. Specifically, D_p approaches the classical value of 2 in the semiclassical regime $\kappa \to \infty$, whereas D_x and D_{xp} vanish in that limit.

5. Pointer states of collisional decoherence

In the previous chapter, I considered the one-dimensional version of QBM and, among other things, I identified the corresponding pointer states. As discussed in Section 4.1.1, the pointer states of three-dimensional QBM can be constructed by a product ansatz of the 1D solutions. However, for other master equations it is, in general, not sufficient to analyze the one-dimensional version in order to make conclusions about solutions in more than one dimension. In Section 3.5.3, I already remarked that the collisional decoherence master equation provides an example for this situation. It is thus not clear how the pointer states of 3D collisional decoherence look like, although their 1D version is well-known from the analysis of Busse and Hornberger [37–39].

In the present chapter, I therefore consider the 3D collisional decoherence master equation and analyze its pointer states, where some of the reasoning is motivated and adopted from Busse [37]. Here, I find that the pointer states are exponentially localized wave packets in phase space that move on Newtonian trajectories, which is analogous to the 1D case [37–39]. This discussion is given in Sections 5.2-5.4. However, there are also significant differences between two- and three-dimensional collisional decoherence and its 1D case, which are derived in Section 5.5. For one thing, the widths of the pointer states are different in all three cases; I estimate them by approximating the pointer states by Gaussian states. For another thing, in two and three dimensions there exist critical regimes when no localized pointer states *are possible*.

In the subsequent chapter, I use the method developed in this chapter for estimating the pointer state widths applying it to a more complicated master equation that I derive from the quantum linear Boltzmann equation.

5.1. Definition of the NLPSE

The master equation of collisional decoherence was already discussed in Section 3.5, where the corresponding Hamiltonian and the Lindblad operator is introduced. According to Eqs. (3.86) and (3.84) they read

$$\begin{aligned} \hat{\mathsf{H}}_0 &= \frac{\hat{\mathbf{p}}^2}{2m}, \\ \hat{\mathsf{L}}_{\boldsymbol{q}} &= \sqrt{\gamma G(\boldsymbol{q})}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar}. \end{aligned} \tag{5.1}$$

It is then straightforward to derive the accompanied NLPSE of collisional decoherence in d dimensions from the general form (3.96),

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi_t\rangle = \hat{\mathsf{N}}[\psi_t]|\psi_t\rangle = \left[\frac{1}{2\mathrm{i}\hbar m}\left(\hat{\mathbf{p}}^2 - \overline{\boldsymbol{p}^2}\right) + \gamma\int \mathrm{d}\boldsymbol{q}\, G(\boldsymbol{q})\langle\psi_t|\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar}|\psi_t\rangle\left(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar} - \langle\psi_t|\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\hat{\mathbf{x}}/\hbar}|\psi_t\rangle\right)\right]|\psi_t\rangle. \tag{5.2}$$

Here, the integration over $\boldsymbol{q}$ is done in d dimensions with $\mathrm{d}\boldsymbol{q} = \mathrm{d}q_1 \ldots \mathrm{d}q_d$. As a most simple and generic momentum kick distribution, I assume $G(\boldsymbol{q})$ to be a normalized Gaussian centered around $\boldsymbol{q} = 0$ with variance σ_G^2,

$$G(\boldsymbol{q}) = \frac{1}{\left(2\pi\sigma_G^2\right)^{d/2}}\mathrm{e}^{-\boldsymbol{q}^2/2\sigma_G^2}. \tag{5.3}$$

For the following derivations, it is convenient to introduce dimensionless units defined by the time, length, and momentum scales

$$\mathrm{T} = \frac{1}{\gamma}, \quad \mathrm{L} = \frac{\hbar}{\sigma_G}, \quad \mathrm{P} = \sigma_G. \tag{5.4}$$

By introducing the single dimensionless parameter

$$\zeta = \frac{\sigma_G^2}{\hbar m\gamma}, \tag{5.5}$$

and the Fourier transform of the momentum kick distribution in dimensionless units

$$\begin{aligned}\tilde{G}(\boldsymbol{x}) &= \int \mathrm{d}\boldsymbol{q}\, G(\boldsymbol{q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}} \\ &= \mathrm{e}^{-\boldsymbol{x}^2/2},\end{aligned} \tag{5.6}$$

one can then write the NLPSE (5.2) in position representation. It reads

$$\frac{\partial}{\partial t}\psi_t(\boldsymbol{x}) = \left(-\frac{\zeta}{2\mathrm{i}}\left(\nabla^2 + \overline{\boldsymbol{p}^2}\right) + \Lambda\left[|\psi_t|^2\right](\boldsymbol{x})\right)\psi_t(\boldsymbol{x}), \tag{5.7}$$

with the localizing term

$$\Lambda\left[|\psi_t|^2\right](\boldsymbol{x}) = \left(|\psi_t|^2 * \tilde{G}\right)(\boldsymbol{x}) - \int \mathrm{d}\boldsymbol{y}\,\left(|\psi_t|^2 * \tilde{G}\right)(\boldsymbol{y})\,|\psi_t(\boldsymbol{y})|^2, \tag{5.8}$$

and the convolution of two functions $(a * b)(\boldsymbol{x}) \equiv \int \mathrm{d}\boldsymbol{y}\, a(\boldsymbol{y})b(\boldsymbol{x} - \boldsymbol{y})$. Notice that the canonical commutator has the form $[\hat{\mathrm{x}}_j, \hat{\mathrm{p}}_k] = \mathrm{i}\delta_{jk}$ in the units (5.4) and the position representation of the momentum operator reads $\langle\boldsymbol{x}|\hat{\mathbf{p}}|\Phi\rangle = -\mathrm{i}\nabla\Phi(\boldsymbol{x})$, both being independent of the parameter ζ.

A *soliton-like solution* $|\pi_t\rangle$, i.e. a pointer state, of the NLPSE is characterized by a wave function moving around in phase space with constant shape. In position representation, this leads to the time dependence $|\pi_t(\boldsymbol{x})| = f(\boldsymbol{x} - \boldsymbol{z}_t)$ with a non-negative function $f(\boldsymbol{x})$ and $\boldsymbol{z}_t$ denoting the time-dependent position of the soliton. Introducing the real function $g(\boldsymbol{x}, t)$, which characterizes the phase of the soliton and, in general, may depend on time, one gets

$$\pi_t(\boldsymbol{x}) = f\left(\boldsymbol{x} - \boldsymbol{z}_t\right) \mathrm{e}^{\mathrm{i}g(\boldsymbol{x},t)}. \tag{5.9}$$

In the following two sections, I show that the soliton moves on trajectories in phase space as given by Newton's laws and that it is exponentially localized.

5.2. The resting soliton

Let us first consider a soliton that does not move in phase space, i.e. its momentum expectation vanishes. According to Eq. (5.9), it is written

$$\pi'_t(\boldsymbol{x}) = f(\boldsymbol{x})\mathrm{e}^{\mathrm{i}g'(\boldsymbol{x},t)}. \tag{5.10}$$

The phase function $g'(\boldsymbol{x}, t)$ is now further characterized by inserting the soliton into the NLPSE (5.7). For this, one first calculates the time derivative and the Laplacian of the soliton (5.10),

$$\begin{aligned} \frac{\partial}{\partial t}\pi'_t(\boldsymbol{x}) &= \mathrm{i}f\dot{g}'\mathrm{e}^{\mathrm{i}g'}, \\ \nabla^2\pi'_t(\boldsymbol{x}) &= \left(\nabla^2 f + \mathrm{i}f\nabla^2 g' + 2\mathrm{i}\nabla f\cdot\nabla g' - f\left(\nabla g'\right)^2\right)\mathrm{e}^{\mathrm{i}g'}, \end{aligned} \tag{5.11}$$

with the abbreviations $f \equiv f(\boldsymbol{x})$, $g' \equiv g'(\boldsymbol{x}, t)$, and $\dot{g}' \equiv \partial g'/\partial t$. The NLPSE (5.7) then reads

$$\mathrm{i}f\dot{g}' = -\frac{\zeta}{2\mathrm{i}}\left(\nabla^2 f + \mathrm{i}f\nabla^2 g' + 2\mathrm{i}\nabla f\cdot\nabla g' - f\left(\nabla g'\right)^2 + f\overline{\boldsymbol{p}^2}\right) + f\Lambda\left[f^2\right](\boldsymbol{x}). \tag{5.12}$$

This equation is now analysed by dividing it into two separate equations for its real and imaginary part, respectively, which read

$$\begin{aligned} \Lambda\left[f^2\right](\boldsymbol{x}) &= \frac{\zeta}{2}\left(\nabla + \nabla\ln f^2\right)\cdot\nabla g', \\ \frac{\zeta}{2}\left(\frac{\nabla^2 f}{f} + \sum_{i=1}^{d}\mathrm{Var}[p_i]\right) &= \dot{g}' + \frac{\zeta}{2}\left(\nabla g'\right)^2, \end{aligned} \tag{5.13}$$

where $\sum_{i=1}^{d}\mathrm{Var}[p_i] = \overline{\boldsymbol{p}^2}$ denotes the sum of the cartesian components of the momentum variance. Because one considers a soliton here, which is defined by a fixed shape, the variance is constant in time.

In Eqs. (5.13), I ordered the terms in a way that the left-hand sides are independent of time; consequently, this imposes a time independence on the right-hand sides, too.

From the first equation of (5.13), one infers that the second factor in the scalar product has to be independent of time, meaning

$$\nabla \dot{g}' = 0. \tag{5.14}$$

This leads to the structure,

$$g'(\boldsymbol{x}, t) = \phi(\boldsymbol{x}) + \chi'(t), \tag{5.15}$$

of the phase function. The requirement of time independence of the right-hand side of the second equation of (5.13) leads to the equation

$$\ddot{g}' + \zeta \nabla g' \cdot \nabla \dot{g}' = 0. \tag{5.16}$$

By that, one can restrict the time dependence of $\chi'(t)$ and gets

$$g'(\boldsymbol{x}, t) = \phi(\boldsymbol{x}) + \chi_1 t, \tag{5.17}$$

with a constant χ_1.

5.3. Soliton dynamics

Coming back to the general case of a soliton (5.9) that moves in phase space, I proceed to determine the soliton's trajectory given by $\boldsymbol{z}_t$. Motivated by the phase function of the resting soliton, Eq. (5.17), I make an ansatz for the phase function of a moving soliton,

$$g(\boldsymbol{x}, t) = \phi(\boldsymbol{x} - \boldsymbol{z}_t) + (\boldsymbol{x} - \boldsymbol{z}_t) \cdot \overline{\boldsymbol{p}} + \chi(t), \tag{5.18}$$

where $\phi(\boldsymbol{x})$ is the spatial dependence of the resting soliton's phase function, $\overline{\boldsymbol{p}}$ is the, in general, time-dependent momentum expectation value, and $\chi(t)$ is a time-dependent function. Note that, at this stage, the trajectory $\boldsymbol{z}_t$ is an arbitrary function of time with the restriction that $\dot{\boldsymbol{z}}_t = \zeta \overline{\boldsymbol{p}}$; in the following derivations it will turn out that the momentum is a constant in time. In this sense, the ansatz (5.18) is qualitatively different from the one given for the 1D model in [37], where a constant momentum is assumed from the beginning.

Along the same lines as in the previous section, one calculates the derivatives of the soliton (5.9), where the Laplacian has the same structure as in Eqs. (5.11) and the time derivative reads

$$\frac{\partial}{\partial t} \pi_t(\boldsymbol{x}) = (-\dot{\boldsymbol{z}}_t \cdot \nabla f + \mathrm{i} f \dot{g})\, \mathrm{e}^{\mathrm{i}g}. \tag{5.19}$$

with the abbreviations $f \equiv f(\boldsymbol{x} - \boldsymbol{z}_t)$ and $g \equiv g(\boldsymbol{x}, t)$ and the dot indicating the temporal derivative. Notice that f is now time-dependent through its argument, in contrast to the above case of the resting soliton. In a next step, one inserts the time derivative and the Laplacian into the NLPSE (5.7) and takes the imaginary part of the equation, which yields

$$\frac{\zeta}{2} \left(\frac{\nabla^2 f}{f} + \sum_{i=1}^{d} \mathrm{Var}[p_i] \right) = \dot{g} + \frac{\zeta}{2} \left((\nabla g)^2 - \overline{\boldsymbol{p}}^2 \right). \tag{5.20}$$

To bring Eq. (5.20) into a suitable form, I make use of the ansatz (5.18) and evaluate the derivatives of the phase function,

$$\begin{aligned} \dot{g} &= -\dot{\boldsymbol{z}}_t \cdot (\nabla\phi + \overline{\boldsymbol{p}}) + (\boldsymbol{x} - \boldsymbol{z}_t) \cdot \dot{\overline{\boldsymbol{p}}} + \dot{\chi}(t), \\ \nabla g &= \nabla\phi + \overline{\boldsymbol{p}}, \end{aligned} \tag{5.21}$$

with $\phi \equiv \phi(\boldsymbol{x} - \boldsymbol{z}_t)$. Equation (5.20) then attains the form,

$$\begin{aligned} \frac{\zeta}{2}\left(\frac{\nabla^2 f}{f} + \sum_{i=1}^{d} \mathrm{Var}[p_i]\right) &= \frac{\zeta}{2}(\nabla\phi)^2 + \nabla\phi \cdot (\zeta\overline{\boldsymbol{p}} - \dot{\boldsymbol{z}}_t) + (\boldsymbol{x} - \boldsymbol{z}_t) \cdot \dot{\overline{\boldsymbol{p}}} - \dot{\boldsymbol{z}}_t \cdot \overline{\boldsymbol{p}} + \dot{\chi}(t). \\ &= \frac{\zeta}{2}(\nabla\phi)^2 + (\boldsymbol{x} - \boldsymbol{z}_t) \cdot \dot{\overline{\boldsymbol{p}}} - \zeta\overline{\boldsymbol{p}}^2 + \dot{\chi}(t), \end{aligned} \tag{5.22}$$

where the second line is obtained by using $\dot{\boldsymbol{z}}_t = \zeta\overline{\boldsymbol{p}}$. I simplify this equation by exploiting the fact that the resting soliton is a solution of the NLPSE. From the second equation of (5.13) together with the phase function (5.17) of the resting soliton, one therefore gets

$$\frac{\zeta}{2}\left(\frac{\nabla^2 f}{f} + \sum_{i=1}^{d} \mathrm{Var}[p_i]\right) = \frac{\zeta}{2}(\nabla\phi)^2 + \chi_1, \tag{5.23}$$

for the resting soliton. Inserting this into Eq. (5.22), finally gives

$$(\boldsymbol{x} - \boldsymbol{z}_t) \cdot \dot{\overline{\boldsymbol{p}}} + \dot{\chi}(t) = \zeta\overline{\boldsymbol{p}}^2 + \chi_1. \tag{5.24}$$

Since the equation has to hold for every $\boldsymbol{x}$, the momentum has to be constant,

$$\dot{\overline{\boldsymbol{p}}} = 0, \tag{5.25}$$

which leads to the phase

$$\chi(t) = \left(\zeta\overline{\boldsymbol{p}}^2 + \chi_1\right) t. \tag{5.26}$$

Thus, the phase function of a moving soliton can be written as

$$g(\boldsymbol{x}, t) = \phi(\boldsymbol{x} - \boldsymbol{z}_t) + (\boldsymbol{x} - \boldsymbol{z}_t) \cdot \overline{\boldsymbol{p}} + \left(\zeta\overline{\boldsymbol{p}}^2 + \chi_1\right) t, \tag{5.27}$$

with a constant momentum $\overline{\boldsymbol{p}}$, meaning that the soliton moves *uniformly* in space.

External potential So far, the discussion applied to a free particle without external fields. However, the above derivation naturally extends to the case of a constant force, which is implemented via the potential

$$V(\boldsymbol{x}) = -\boldsymbol{k} \cdot \boldsymbol{x}. \tag{5.28}$$

To incorporate the effect of the potential, the term $\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{x} - \overline{\boldsymbol{x}})\, \psi_t(\boldsymbol{x})$ has to be added to the right-hand side of the NLPSE (5.7). Following exactly the derivation for the free

case, one calculates the imaginary part of the NLPSE, which equals Eq. (5.22) except that the right-hand side is extended by the term $-\boldsymbol{k}\cdot(\boldsymbol{x}-\overline{\boldsymbol{x}})$:

$$\frac{\zeta}{2}\left(\frac{\nabla^2 f}{f}+\sum_{i=1}^{d}\mathrm{Var}[p_i]\right)=\frac{\zeta}{2}\left(\nabla\phi\right)^2+(\boldsymbol{x}-\boldsymbol{z}_t)\cdot\dot{\overline{\boldsymbol{p}}}-\zeta\overline{\boldsymbol{p}}^2+\dot{\chi}(t)-\boldsymbol{k}\cdot(\boldsymbol{x}-\overline{\boldsymbol{x}})\,. \quad (5.29)$$

Again, exploiting that the resting soliton is a solution of the free NLPSE, see Eq. (5.23), one arrives at

$$(\boldsymbol{x}-\boldsymbol{z}_t)\cdot\dot{\overline{\boldsymbol{p}}}+\dot{\chi}(t)=\boldsymbol{k}\cdot(\boldsymbol{x}-\overline{\boldsymbol{x}})+\zeta\overline{\boldsymbol{p}}^2+\chi_1. \quad (5.30)$$

Matching the spatial dependencies on both sides and using $\boldsymbol{z}_t=\overline{\boldsymbol{x}}$ leads to a constantly accelerated soliton,

$$\dot{\overline{\boldsymbol{p}}}=\boldsymbol{k}, \quad (5.31)$$

and to the phase

$$\dot{\chi}(t)=\zeta\overline{\boldsymbol{p}}^2+\chi_1. \quad (5.32)$$

In accordance with Newton's laws, applying a linear potential to the system leads to a *uniformly accelerated* soliton with phase function $g(\boldsymbol{x},t)$ from Eq. (5.18) and $\chi(t)$ according to Eq. (5.32). For nonlinear potentials, following the argument in [37–39], the soliton moves also approximately on the Newtonian trajectories as long as the potential is linearizable over the spatial extension of the soliton.

5.4. Asymptotic form of the soliton

Although the complete form of the shape $f(\boldsymbol{x})$ is not analytically tractable, one can show that its tails decay exponentially, i.e. the solitons are exponentially localized. Here, I can follow the argumentation of the 1D calculation [37–39], in which one explores the tails of the resting soliton (5.10). At asymptotically large positions, $|\boldsymbol{x}|\to\infty$, the convolution in the localization term (5.8) vanishes and one is left with the state-dependent positive constant

$$\Lambda\left[\left|\pi_t'\right|^2\right](\boldsymbol{x})\to-\Lambda_{\pi'}. \quad (5.33)$$

In the limit $|\boldsymbol{x}|\to\infty$, the NLPSE (5.12) of the resting soliton therefore reads

$$\begin{aligned}\mathrm{i}f(\boldsymbol{x})\chi_1=&-\Lambda_{\pi'}f(\boldsymbol{x})\\&-\frac{\zeta}{2\mathrm{i}}\left[\nabla^2 f(\boldsymbol{x})-f(\boldsymbol{x})\left[\nabla\phi(\boldsymbol{x})\right]^2+2\mathrm{i}\nabla f(\boldsymbol{x})\cdot\nabla\phi(\boldsymbol{x})+\mathrm{i}f(\boldsymbol{x})\nabla^2\phi(\boldsymbol{x})+f(\boldsymbol{x})\mathrm{V}_{\pi'}\right],\end{aligned} \quad (5.34)$$

where $\mathrm{V}_{\pi'}=\sum_{j=1}^{d}\mathrm{Var}(p_j')$ is the sum of the cartesian components of the momentum variance of state π'. The real and imaginary parts of Eq. (5.34) yield two coupled differential equations,

$$\begin{aligned}-\frac{\Lambda_{\pi'}}{\zeta}&=\nabla\ln f(\boldsymbol{x})\cdot\nabla\phi(\boldsymbol{x})+\frac{1}{2}\nabla^2\phi(\boldsymbol{x}),\\\left(\frac{2}{\zeta}\chi_1-\mathrm{V}_{\pi'}\right)&=\nabla^2\ln f(\boldsymbol{x})+\left[\nabla\ln f(\boldsymbol{x})\right]^2-\left[\nabla\phi(\boldsymbol{x})\right]^2,\end{aligned} \quad (5.35)$$

for which a normalizable isotropic solution is given by the exponential,

$$\begin{aligned} f(\boldsymbol{x}) &= A\mathrm{e}^{-\alpha|\boldsymbol{x}|}, \\ \phi(\boldsymbol{x}) &= \frac{\Lambda_{\pi'}}{\zeta\alpha}\,|\boldsymbol{x}|\,, \end{aligned} \tag{5.36}$$

where A is a normalization constant and

$$\alpha = \frac{1}{\sqrt{\zeta}}\sqrt{\chi_1 - \frac{\zeta}{2}V_{\pi'} + \sqrt{\Lambda_{\pi'}^2 + \left(\chi_1 - \frac{\zeta}{2}V_{\pi'}\right)^2}}. \tag{5.37}$$

5.5. Widths of the soliton

Along with their shape, the position and momentum variances are an important characteristic of the soliton.[1] It is straightforward to derive equations of motion for any (time-independent) hermitian operator $\hat{\mathsf{A}}$ from the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{A} = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t|\hat{\mathsf{A}}|\psi_t\rangle = \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t|\right)\hat{\mathsf{A}}|\psi_t\rangle + \langle\psi_t|\hat{\mathsf{A}}\left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi_t\rangle\right) = 2\mathrm{Re}\left\{\langle\psi_t|\hat{\mathsf{A}}\hat{\mathsf{N}}[\psi_t]|\psi_t\rangle\right\}, \tag{5.38}$$

where the NLPSE (5.2) is used. However, for the position and momentum variances, these equations of motion do not form a closed set. Nonetheless, suitable differential equations for the variances of the soliton can be derived by approximating it by a Gaussian wave packet with variable variances. For the discussion of the widths, it is sufficient to consider a resting wave packet, $\overline{\boldsymbol{x}} = \overline{\boldsymbol{p}} = 0$. Moreover, the state is assumed to be spherically symmetric and can thus be written as

$$\psi(\boldsymbol{x}) = \frac{1}{(2\pi V_x)^{d/4}}\exp\left(-\frac{1-\mathrm{i}C_{xp}}{4V_x}\boldsymbol{x}^2\right), \tag{5.39}$$

where the parameter d denotes the dimension and $V_x = \overline{x_j^2}$ and $C_{xp} = \overline{\{x_j, p_j\}}$ are the position variance and the covariance. Notice that the variances are equal to the second moment in the present case of vanishing first moments and due to the state's spherical symmetry they can be calculated with any component of the vector operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$. In addition, the variances in position and momentum space and the covariance are related via

$$4V_xV_p = 1 + C_{xp}^2, \tag{5.40}$$

due to the Gaussianity of the state (cf. Eq. (3.14) in Section 3.1.3). As usual, all expectation values are time-dependent due to the time dependence of the state, which I omit to write down explicitly for brevity.

[1] Since the width of the soliton follows from the variance by taking the square root, I will use the two terms interchangeably.

5.5.1. Position variance

A differential equation for the position variance, $V_x = \overline{x_j^2}$ with arbitrary $j \in \{1, \ldots, d\}$, is derived directly from Eq. (5.38). It reads

$$\frac{\mathrm{d}}{\mathrm{d}t} V_x = \frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{ham}} + \frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{loc}}, \tag{5.41}$$

with the Hamiltonian and the localization contributions

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{ham}} &= 2\mathrm{Re}\left\{ \int \mathrm{d}\boldsymbol{x} \psi(\boldsymbol{x})^* x_j^2 \frac{\mathrm{i}\zeta}{2} \left(\nabla^2 - \overline{\boldsymbol{p}^2} \right) \psi(\boldsymbol{x}) \right\}, \\ \frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{loc}} &= 2\mathrm{Re}\left\{ \int \mathrm{d}\boldsymbol{x} \, |\psi(\boldsymbol{x})|^2 \, x_j^2 \left[\left(|\psi|^2 * \tilde{G} \right)(\boldsymbol{x}) - \int \mathrm{d}\boldsymbol{y} \left(|\psi|^2 * \tilde{G} \right)(\boldsymbol{y}) \, |\psi(\boldsymbol{y})|^2 \right] \right\}. \end{aligned} \tag{5.42}$$

Hamiltonian contribution The second summand of the Hamiltonian contribution contains the expectation value $\overline{\boldsymbol{p}^2}$ and therefore vanishes because the integral is purely real. This also holds for any hermitian operator not just for $\hat{\mathrm{x}}_j^2$.

The first summand of the Hamiltonian part, however, does not vanish and in order to calculate the occuring integral, one makes use of the Laplacian of the Gaussian state in Eqs. (3.15) to get

$$\nabla^2 \psi(\boldsymbol{x}) = \frac{1 - \mathrm{i}C_{xp}}{2V_x} \left(\frac{1 - \mathrm{i}C_{xp}}{2V_x} \boldsymbol{x}^2 - d \right) \psi(\boldsymbol{x}). \tag{5.43}$$

The integration is then carried out straightforwardly by evaluation of Gaussian integrals and gives

$$\frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{ham}} = \zeta \mathrm{Re}\left\{ \mathrm{i} \left[(1 - \mathrm{i}C_{xp})^2 \frac{d+2}{4} - (1 - \mathrm{i}C_{xp}) \frac{d}{2} \right] \right\}. \tag{5.44}$$

Upon using the identities

$$\begin{aligned} \mathrm{Re}\left\{ \mathrm{i}a \right\} &= -\mathrm{Im}\left\{ a \right\}, \\ \mathrm{Im}\left\{ (1 - \mathrm{i}C_{xp})^2 \right\} &= -2C_{xp}, \end{aligned} \tag{5.45}$$

the real part of Eq. (5.44) is easily calculated. One arrives at the Hamiltonian contribution

$$\frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{ham}} = \zeta C_{xp}. \tag{5.46}$$

Localization contribution For the derivation of the localization part $\mathrm{d}V_{x,\mathrm{loc}}/\mathrm{d}t$ from Eqs. (5.42), it is useful to evaluate the two summands in square brackets in advance. The first one consists of the convolution of the absolute value $|\psi(\boldsymbol{x})|^2$ with the Fourier

transform of the momentum kick distribution $\tilde{G}(\boldsymbol{x}) = \exp\left(-\boldsymbol{x}^2/2\right)$, see Eq. (5.6). It gives the non-normalized Gaussian function

$$\begin{aligned}\left(|\psi|^2 * \tilde{G}\right)(\boldsymbol{x}) &= \frac{1}{(2\pi V_x)^{d/2}} \int \mathrm{d}\boldsymbol{y} \exp\left(-\frac{\boldsymbol{y}^2}{2V_x} - \frac{(\boldsymbol{x}-\boldsymbol{y})^2}{2}\right) \\ &= \frac{1}{(1+V_x)^{d/2}} \exp\left(-\frac{\boldsymbol{x}^2}{2\,(1+V_x)}\right). \end{aligned} \tag{5.47}$$

The second term of the localization part of Eqs. (5.42) is gained by integrating $|\psi(\boldsymbol{x})|^2$ over the above convolution (5.47),

$$\begin{aligned}\int \mathrm{d}\boldsymbol{y} \left(|\psi|^2 * \tilde{G}\right)(\boldsymbol{y}) |\psi(\boldsymbol{y})|^2 &= \frac{1}{(2\pi V_x\,(1+V_x))^{d/2}} \int \mathrm{d}\boldsymbol{y} \exp\left(-\frac{\boldsymbol{y}^2}{2\,(1+V_x)} - \frac{\boldsymbol{y}^2}{2V_x}\right) \\ &= \frac{1}{(1+2V_x)^{d/2}}. \end{aligned} \tag{5.48}$$

The integrals in $\mathrm{d}V_{x,\mathrm{loc}}/\mathrm{d}t$ can now be determined and yield the localization contribution

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} V_{x,\mathrm{loc}} &= 2\left(\frac{(1+V_x)\,V_x}{(1+2V_x)^{(d+2)/2}} - \frac{V_x}{(1+2V_x)^{d/2}}\right) \\ &= -\frac{2V_x^2}{(1+2V_x)^{(d+2)/2}}. \end{aligned} \tag{5.49}$$

Finally, by combining the Hamiltonian and the localization parts from Eqs. (5.46) and (5.49), one gets the equation of motion of the position variance

$$\frac{\mathrm{d}}{\mathrm{d}t} V_x = \zeta C_{xp} - \frac{2V_x^2}{(1+2V_x)^{(d+2)/2}}. \tag{5.50}$$

5.5.2. Momentum variance

The equation of motion for the momentum variance V_p is calculated accordingly by starting with an equation similar to the one for $\mathrm{d}V_x/\mathrm{d}t$. In particular, as Hamiltonian and localization parts one derives

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} V_{p,\mathrm{ham}} &= -2\mathrm{Re}\left\{\int \mathrm{d}\boldsymbol{x}\psi(\boldsymbol{x})^* \frac{\partial^2}{\partial x_j^2} \frac{\mathrm{i}\zeta}{2} \nabla^2 \psi(\boldsymbol{x})\right\}, \\ \frac{\mathrm{d}}{\mathrm{d}t} V_{p,\mathrm{loc}} &= -2\mathrm{Re}\Bigg\{\int \mathrm{d}\boldsymbol{x}\psi(\boldsymbol{x})^* \frac{\partial^2}{\partial x_j^2} \Bigg[\left(|\psi|^2 * \tilde{G}\right)(\boldsymbol{x}) \\ &\qquad - \int \mathrm{d}\boldsymbol{y} \left(|\psi|^2 * \tilde{G}\right)(\boldsymbol{y}) |\psi(\boldsymbol{y})|^2\Bigg] \psi(\boldsymbol{x})\Bigg\}. \end{aligned} \tag{5.51}$$

Hamiltonian contribution Since $\hat{\mathsf{p}}_j^2$ is a hermitian operator I left out the vanishing second summand of the Hamiltonian part, as was already discussed in the calculation for V_x.

The remaining part is computed by taking the second derivative of the Laplacian from Eq. (5.43),

$$\partial_j^2 \nabla^2 \psi(\boldsymbol{x}) = \frac{(1-\mathrm{i}C_{xp})^2}{4V_x^2}\left(d+2-\frac{1-\mathrm{i}C_{xp}}{2V_x}\left(\boldsymbol{x}^2+(d+4)\,x_j^2\right)+\frac{(1-\mathrm{i}C_{xp})^2}{4V_x^2}\boldsymbol{x}^2 x_j^2\right)\psi(\boldsymbol{x}). \tag{5.52}$$

Upon integrating this expression, one gets a vanishing Hamiltonian contribution

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V_{p,\mathrm{ham}} &= \zeta \mathrm{Im}\left\{\frac{d+2}{4V_x^2}(1-\mathrm{i}C_{xp})^2\left(1-(1-\mathrm{i}C_{xp})+(1-\mathrm{i}C_{xp})^2\,\frac{1}{4}\right)\right\}\\ &= 0,\end{aligned} \tag{5.53}$$

where one uses the identities (5.45) complemented by

$$\begin{aligned}\mathrm{Im}\left\{(1-\mathrm{i}C_{xp})^3\right\} &= -3C_{xp}+C_{xp}^3,\\ \mathrm{Im}\left\{(1-\mathrm{i}C_{xp})^4\right\} &= -4C_{xp}+4C_{xp}^3.\end{aligned} \tag{5.54}$$

Localization contribution To calculate the localization part, I use the solutions (5.47) and (5.48) of the previous section for the two terms in square brackets in Eqs. (5.51). After computing the second derivative, the localization part reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V_{p,\mathrm{loc}} = -2\mathrm{Re}\Bigg\{&\int \mathrm{d}\boldsymbol{x}\,|\psi(\boldsymbol{x})|^2\left(|\psi|^2 * \tilde{G}\right)(\boldsymbol{x})\\ &\left[\left(\frac{1}{(1+V_x)^2}+\frac{1-\mathrm{i}C_{xp}}{V_x\,(1+V_x)}+\frac{(1-\mathrm{i}C_{xp})^2}{4V_x^2}\right)x_j^2-\frac{1}{1+V_x}-\frac{1-\mathrm{i}C_{xp}}{2V_x}\right]\Bigg\}\\ &+2\mathrm{Re}\left\{\int \mathrm{d}\boldsymbol{x}\,|\psi(\boldsymbol{x})|^2\,\frac{1-\mathrm{i}C_{xp}}{2\,(1+2V_x)^{d/2}\,V_x}\left(\frac{1-\mathrm{i}C_{xp}}{2V_x}x_j^2-1\right)\right\}.\end{aligned} \tag{5.55}$$

These integrals are evaluated analogous to those that lead to the localization contribution (5.49) of V_x and one obtains after some algebra the localization contribution, which coincides with the equation of motion of the momentum variance,

$$\frac{\mathrm{d}}{\mathrm{d}t}V_p = \frac{\mathrm{d}}{\mathrm{d}t}V_{p,\mathrm{loc}} = \frac{1-C_{xp}^2}{2\,(1+2V_x)^{(d+2)/2}}. \tag{5.56}$$

5.5.3. Stationary variances in various dimensions

The differential equations for the variances, Eqs. (5.50) and (5.56), depend on the dimension d of the system. As we shall see in this section, this has crucial implications on the existence of stationary variances and solitons.

Stationary solutions are found by setting $\mathrm{d}V_{x,\mathrm{ps}}/\mathrm{d}t = \mathrm{d}V_{p,\mathrm{ps}}/\mathrm{d}t = 0$, which leads to the equations

$$\begin{aligned} 0 &= \zeta C_{xp,\mathrm{ps}} - \frac{2V_{x,\mathrm{ps}}^2}{(1+2V_{x,\mathrm{ps}})^{(d+2)/2}}, \\ 0 &= \frac{1 - C_{xp,\mathrm{ps}}^2}{2\,(1+2V_{x,\mathrm{ps}})^{(d+2)/2}}, \end{aligned} \tag{5.57}$$

where the subscript "ps" stands for "pointer state" and denotes the stationary values. At first, one sees that Eqs. (5.57) can only be fulfilled for

$$C_{xp,\mathrm{ps}} = 1. \tag{5.58}$$

The remaining equation can be understood as a mapping from the width $V_{x,\mathrm{ps}}$ to ζ,

$$\zeta(V_{x,\mathrm{ps}}) = \frac{2V_{x,\mathrm{ps}}^2}{(1+2V_{x,\mathrm{ps}})^{(d+2)/2}}. \tag{5.59}$$

Figure 5.1(a) shows the inverted relation (5.59), i.e. the soliton variance $V_{x,\mathrm{ps}}$ as function of the parameter ζ, in a double logarithmic plot for dimensions $d = 1$, 2, and 3. Moreover, I inserted the theoretical prediction for the pointer state width as calculated in [37, 39], which is applicable for large ζ only. Figure 5.1(b) presents the numerical values of the position variance as obtained by an implementation of the NLPSE (5.2). The analytic expressions from the localization model are shown as dashed lines for comparison. One finds that the analytic results are in very good agreement with the numerics for all dimensions and all ranges of ζ.

Interestingly, for small ζ-values all three curves coincide and it is remarkable that only in the one-dimensional version one gets a stationary solution for every ζ. In two and three dimensions there exist critical ζ-values above which no soliton-like solutions, i.e. no pointer states exist. From Eq. (5.59) one infers that in the two-dimensional case the critical value of the dimensionless parameter is

$$\zeta_{\mathrm{crit}}^{\mathrm{2D}} = \frac{1}{2}, \tag{5.60}$$

with the variance growing above all bounds, $V_{x,\mathrm{ps}}^{\mathrm{2D}}(\zeta_{\mathrm{crit}}^{\mathrm{2D}}) \to \infty$. Analogously, in three dimensions one gets

$$\zeta_{\mathrm{crit}}^{\mathrm{3D}} = \frac{8}{5^{5/2}} \approx 0.143, \tag{5.61}$$

which yields a finite variance limit $V_{x,\mathrm{ps}}^{\mathrm{3D}}(\zeta_{\mathrm{crit}}^{\mathrm{3D}}) = 2$.

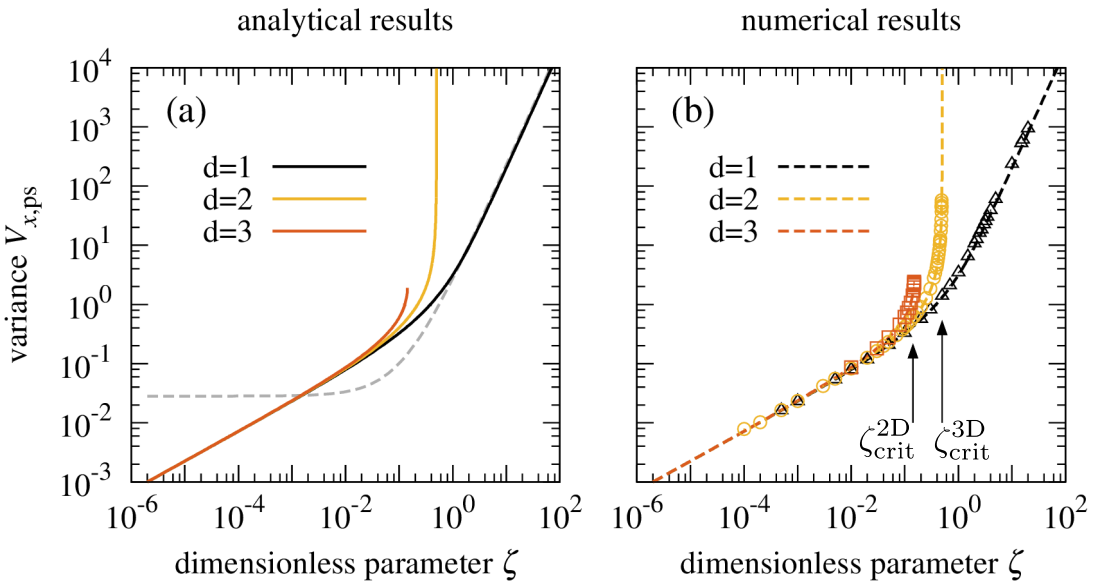

Figure 5.1.: Dependence of the soliton width $V_{x,\mathrm{ps}}$ on the parameter ζ. Panel (a) shows the analytic approximation as obtained by inverting Eq. (5.59). The grey dashed line gives the prediction from the 1D model in [37], which is applicable for large ζ only. Panel (b) presents the position variance obtained by a numerical implementation of the NLPSE (5.2). One observes that in all considered dimensions and for all ζ the calculated widths are in very good agreement with the numerically obtained ones.

5.5.4. Discussion

In this last part of the present chapter, I presented a method to estimate the width of the pointer states of collisional decoherence by approximating them with Gaussian states. By propagating these Gaussian states according to the NLPSE, I calculated the equations of motion for the position an momentum variances and looked for their stationary solutions.

From Fig. 5.1(a), one observes that the present model extends nontrivially the works of Busse and Hornberger [37–39]. Their model for the width of the 1D pointer state is based on the heuristic picture of a freely dispersing wave packet that is spatially localized by environmental kicks. Upon averaging over this process of free dispersion and localization with the distribution of the kicks, one arrives at a model with one free parameter. Fitting to the numerical data at large ζ yields the grey dashed line in Fig. 5.1(a). In contrast to that, the present localization model based on Gaussian states gives a parameter-free prediction of the width in all three dimensions, see Eq. (5.59). As one infers from a comparison with the numerical data in Fig. 5.1, its applicability goes over the whole range of ζ.

A most interesting fact thus revealed is the existence of critical parameter values in two and three dimensions, see Eqs. (5.60) and (5.61), above which no pointer states exist. This is an unexpected finding since it is in sharp contrast to the 1D behavior and cannot be deduced from a 1D analysis. It is therefore evident that the multidimensional properties of the unraveling of collisional decoherence are not obtained by a simple extrapolation of the 1D results, as is suggested in [37–39].

The dependence of the width equation (5.59) on the dimension d enters via its denominator, which in turn attains its particular form from the assumed Gaussian kick distribution $G(\boldsymbol{Q})$ as seen in Eqs. (5.47) and (5.48). Taking as kick distributions non-Gaussian functions or functions derived on microscopic grounds, may thus still allow pointer states for all parameter values. Moreover, incorporating dissipative effects into the collisional decoherence model, also gives a more realistic description of the open system dynamics and one might hope that this removes or reduces the critical behavior of the pointer state width encountered in this chapter.

I discuss both points in the following chapter, where I will derive a dissipative Lindblad master equation on basis of the quantum linear Boltzmann equation. In its non-dissipative limit, this new master equation gives the collisional decoherence model. To estimate the pointer state widths of that master equation, I make use of the Gaussian localization model, which I introduced and proved valuable here.

6. Quantum linear Boltzmann equation (QLBE)

In this last chapter, I want to go beyond the limits of the master equations discussed in the previous two chapters, namely quantum Brownian motion (QBM) and collisional decoherence. QBM serves as a paradigmatic model for dissipative quantum systems, however, it is only linear in its environmental coupling. Collisional decoherence, on the other hand, is a model for a particle of infinite mass that incorporates the environmental coupling via a scattering analysis and therefore exhibits Lindblad operators with an exponential dependence on the position operator. Due to the infinite mass limit, which is drawn with respect to the gas particle mass, this model does not describe dissipation effects.

These "drawbacks" may be tackled by turning to a dissipative Lindblad master equation derived on microscopic grounds: the quantum linear Boltzmann equation (QLBE). It describes a marker particle under influence of a gas environment using the elastic scattering amplitudes associated to the interaction potential as input [25]. As such, it incorporates the environmental coupling in a non-perturbative way. After introducing the equation itself, I show in Section 6.2 that both the QBM and collisional decoherence master equation can be obtained as limiting cases of the QLBE. In particular, the latter being the non-dissipative limit of the QLBE, which one arrives at by sending the ratio of the gas to marker particle masses to zero, i.e. $m/M \to 0$. Consequently, an expansion of the Lindblad operator to first order in m/M yields a systematic extension of collisional decoherence. In Section 6.3, I derive the Lindblad operator in this mass approximation and discuss some properties of the corresponding master equation in the subsequent two sections. For one thing, in Section 6.4, the derivation of the behavior of the first moments of position and momentum as well as their corresponding variances shows that this master equation is dissipative and diffusive. For another thing, the positional decoherence behavior turns out to be similar to the one exhibited in collisional decoherence, which I show in Section 6.5.

Finally, in the last Section 6.6, I elucidate aspects of the associated pointer states by deriving the corresponding NLPSE and estimating the pointer state widths in position and momentum. Here, I draw upon the localization model I derived and tested for the pointer states of collisional decoherence in the previous chapter. In particular, the localization model is based on an approximation of the pointer states by Gaussian states and propagating them according to the NLPSE. I will compare the occuring equation for the pointer state width with the one I derived for collisional decoherence and it turns out that dissipation effects pose a lower bound to the position width but leave the critical behavior of the collisional decoherence model unchanged. However, choosing

a momentum kick distribution that is not Gaussian may lead to pointer states for all parameter values.

6.1. Definition of the QLBE

The QLBE describes non-perturbatively the influence of a gaseous environment on a marker particle [25]. It has the form of a Lindblad master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}[\hat{\mathsf{H}}_0 + \hat{\mathsf{H}}_\mathrm{n}, \rho] + \mathcal{D}\rho, \tag{6.1}$$

with the kinetic energy $\hat{\mathsf{H}}_0 = \hat{\mathbf{P}}^2/(2M)$ of the marker particle, the energy shift $\hat{\mathsf{H}}_\mathrm{n}$ defined below, and the dissipator $\mathcal{D}\rho$ of Lindblad type. In the following, upper case letters refer to the test particle whereas lower case letters refer to gas particle properties.

The dissipator in Eq. (6.1) has the form

$$\mathcal{D}\rho = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \left[\hat{\mathsf{L}}(\boldsymbol{k}_\perp, \boldsymbol{Q})\,\rho\hat{\mathsf{L}}^\dagger(\boldsymbol{k}_\perp, \boldsymbol{Q}) - \frac{1}{2}\left\{\rho, \hat{\mathsf{L}}^\dagger(\boldsymbol{k}_\perp, \boldsymbol{Q})\,\hat{\mathsf{L}}(\boldsymbol{k}_\perp, \boldsymbol{Q})\right\}\right], \tag{6.2}$$

where the five dimensional integration is over all momentum transfers $\boldsymbol{Q}$ and over the gas particle momenta $\boldsymbol{k}_\perp$ being from the plane perpendicular to $\boldsymbol{Q}$, which is denoted by $\boldsymbol{Q}_\perp$. The Lindblad operator is a function of these two momenta as well as of the position and momentum operator $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$:

$$\hat{\mathsf{L}}(\boldsymbol{k}_\perp, \boldsymbol{Q}) = \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\sqrt{\frac{n_\mathrm{gas} m}{m_*^2 Q}}\, f\left(\mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathbf{P}}_\perp\right) - \frac{\boldsymbol{Q}}{2}, \mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathbf{P}}_\perp\right) + \frac{\boldsymbol{Q}}{2}\right) \times \sqrt{\mu\left(\boldsymbol{k}_\perp + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\hat{\mathbf{P}}_\parallel\right)}. \tag{6.3}$$

Here, m and M denote the masses of the gas particles and the test particle, respectively; $m_* = mM/(m+M)$ is the reduced mass and n_gas is the number density of the gas particles. The subscripts $\perp$ and $\parallel$ denote vector components perpendicular and parallel to the momentum transfer $\boldsymbol{Q}$, i.e. $\boldsymbol{P}_\parallel = \boldsymbol{P}\cdot(\boldsymbol{Q}\otimes\boldsymbol{Q})/Q^2$ and $\boldsymbol{P}_\perp = \boldsymbol{P} - \boldsymbol{P}_\parallel$.[1] The function $\mu(\boldsymbol{p})$ describes any stationary distribution function of the gas momenta but in the present analysis it is always chosen to be the Maxwell-Boltzmann distribution

$$\mu(\boldsymbol{p}) = \frac{1}{\left(\pi p_\beta^2\right)^{3/2}}\mathrm{e}^{-\boldsymbol{p}^2/p_\beta^2}, \tag{6.4}$$

where $p_\beta = \sqrt{2m/\beta}$ is the most probable momentum and $\beta = 1/k_\mathrm{B}T$ is the inverse thermal energy at temperature T. $f(\boldsymbol{p}_\mathrm{f}, \boldsymbol{p}_\mathrm{i})$ is the elastic scattering amplitude between

[1] $\boldsymbol{A}\otimes\boldsymbol{B}$ is the dyadic product, with properties $\boldsymbol{C}\cdot(\boldsymbol{A}\otimes\boldsymbol{B}) = (\boldsymbol{C}\cdot\boldsymbol{A})\,\boldsymbol{B}$ and $(\boldsymbol{A}\otimes\boldsymbol{B})\cdot\boldsymbol{C} = \boldsymbol{A}\,(\boldsymbol{B}\cdot\boldsymbol{C})$.

an initial momentum $\boldsymbol{p}_\mathrm{i}$ and a final momentum $\boldsymbol{p}_\mathrm{f}$. It involves in its arguments the relative momenta

$$\mathrm{rel}\,(\boldsymbol{p},\boldsymbol{P}) \equiv m_* \left(\frac{\boldsymbol{p}}{m} - \frac{\boldsymbol{P}}{M}\right). \tag{6.5}$$

Finally, the energy shift induced by the environmental coupling of the master equation (6.1) is defined by

$$\hat{\mathsf{H}}_\mathrm{n} = -2\pi\hbar^2 \frac{n_\mathrm{gas}}{m_*} \int \mathrm{d}\boldsymbol{p}\, \mu(\boldsymbol{p}) \mathrm{Re}\left\{ f\left(\mathrm{rel}\left(\boldsymbol{p},\hat{\mathbf{P}}\right), \mathrm{rel}\left(\boldsymbol{p},\hat{\mathbf{P}}\right)\right)\right\}. \tag{6.6}$$

Due to its complexity, the QLBE is difficult to solve in general. One is therefore tempted to look at limiting cases or to make simplifying approximations in order to improve the understanding of the properties and pointer states of the QLBE. In fact, as we will see in the following and as I already mentioned above, collisional decoherence and QBM are two of the limits of the QLBE. But before coming to that, I make a remark on isotropic scattering processes, which I consider in the remainder of the chapter.

Isotropic scattering processes For isotropic elastic scattering processes, the dependence of $f(\cdot,\cdot)$ on its arguments can be simplified to

$$f\left(\boldsymbol{p}_\mathrm{f},\boldsymbol{p}_\mathrm{i}\right) \equiv f\left(p_\perp, Q\right), \tag{6.7}$$

with the absolute values of the momentum transfer and the perpendicular projection of $\boldsymbol{p}_\mathrm{i,f}$ on $\boldsymbol{Q}$, respectively,

$$\begin{aligned} Q &= |\boldsymbol{Q}| = |\boldsymbol{p}_\mathrm{i} - \boldsymbol{p}_\mathrm{f}|\,, \\ p_\perp &= |\boldsymbol{p}_\perp| = |\boldsymbol{p}_\mathrm{i} + \boldsymbol{p}_\mathrm{f}|\,/2. \end{aligned} \tag{6.8}$$

These two relations can be easily infered by drawing the momenta involved, see Fig. 6.1. Since the orientation of the isosceles triangle spanned by the initial and final relative momenta does not matter for isotropic scattering processes, it is only neccessary to define its aspect ratio. This can be done by two appropriate scalars, e.g. the base of the triangle Q and its corresponding midperpendicular $p_\perp$. Another well-known choice is obtained by giving the vertex angle ϑ and the length of the two accompanying edges $p_\mathrm{i,f} = |\boldsymbol{p}_\mathrm{i,f}|$ along with the demand that the triangle must be isosceles.

In the isotropic case, one can therefore rewrite for the scattering amplitude in the Lindblad operator (6.3),

$$f\left(\mathrm{rel}\left(\boldsymbol{k}_\perp,\hat{\mathbf{P}}_\perp\right) - \frac{\boldsymbol{Q}}{2}, \mathrm{rel}\left(\boldsymbol{k}_\perp,\hat{\mathbf{P}}_\perp\right) + \frac{\boldsymbol{Q}}{2}\right) \equiv f\left(\left|\mathrm{rel}\left(\boldsymbol{k}_\perp,\hat{\mathbf{P}}_\perp\right)\right|, Q\right). \tag{6.9}$$

6.2. Limiting cases

This short review of two limiting cases of the QLBE is motivated by Ref. [25] and the following derivations are also found therein.

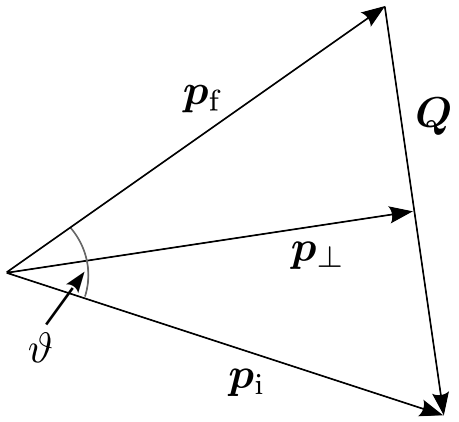

Figure 6.1.: Triangle of momenta for elastic isotropic scattering. $\boldsymbol{p}_{\mathrm{i,f}}$ are the vectors of the initial and final relative momenta between the tracer and the gas particle, $\boldsymbol{p}_\perp$ is their component perpendicular to the momentum transfer $\boldsymbol{Q}$, and ϑ denotes the scattering angle. Energy conservation means that $|\boldsymbol{p}_\mathrm{f}| = |\boldsymbol{p}_\mathrm{i}|$, which is equivalent to $\boldsymbol{p}_\perp$ being the midperpendicular of the triangle; isotropy is reflected by the fact that only the aspect ratio of the triangle is relevant, but not its orientation in space.

6.2.1. Collisional decoherence

In case of a very massive test particle, one can simplify the QLBE (6.1) by assuming the limit $m/M \to 0$. The dependence on the momentum operator vanishes in this case and one arrives at the master equation of collisional decoherence.

In calculating the limit $m/M \to 0$, one first infers for the relative mass that $m_* \to m$, which leads to the relative momenta $\mathrm{rel}\,(\boldsymbol{p}, \boldsymbol{P}) \to \boldsymbol{p}$. The Lindblad operator (6.3) therefore simplifies to

$$\hat{\mathsf{L}}\,(\boldsymbol{k}_\perp, \boldsymbol{Q}) \to \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{x}}/\hbar} \sqrt{\frac{n_\mathrm{gas}}{mQ}} f\,(k_\perp, Q)\, \sqrt{\mu\,(k_\perp, Q)}, \tag{6.10}$$

with

$$\mu(k_\perp, Q) \equiv \mu\left(\boldsymbol{k}_\perp + \frac{\boldsymbol{Q}}{2}\right) = \frac{\mathrm{e}^{-\left(k_\perp^2 + Q^2/4\right)/p_\beta^2}}{\left(\pi p_\beta^2\right)^{3/2}}. \tag{6.11}$$

Equation (6.11) is directly derived by noting that the vectors $\boldsymbol{k}_\perp$ and $\boldsymbol{Q}$ are perpendicular, by construction, and by using the definition (6.4) of the Maxwell–Boltzmann distribution. The distribution of momentum transfers is identified as the integral

$$\gamma G(Q) = \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \frac{n_\mathrm{gas}}{mQ} \left|f\,(k_\perp, Q)\right|^2 \mu\,(k_\perp, Q)\,, \tag{6.12}$$

which then yields the master equation of collisional decoherence

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}_0, \rho\right] + \gamma \int \mathrm{d}\boldsymbol{Q}\, G(Q) \left(\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{x}}/\hbar} \rho \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{x}}/\hbar} - \rho\right). \tag{6.13}$$

Here, the rate γ is determined by the normalization of $G(Q)$. Notice that, in general, $G(\cdot)$ also depends on the orientation of the momentum $\boldsymbol{Q}$; since I considered isotropic scattering processes only, this dependence reduces to the vector's absolute value.

The energy shift $\hat{\mathsf{H}}_\mathrm{n}$ from Eq. (6.6) becomes independent of the momentum operator in this limit and due to its appearance inside the commutator only, it makes no contribution to the master equation (6.13).

6.2.2. Quantum Brownian motion

The limit of quantum Brownian motion (QBM) is a little bit more subtle to draw than that of collisional decoherence. The first approximation to make is that the test particle is much heavier than the gas particles such that the ratio of their masses m/M is small but nonzero. Additionally, the state of the test particle should be close to a thermal state, i.e. in momentum representation, one requires $\langle \boldsymbol{P}|\rho|\boldsymbol{P}'\rangle \approx 0$ for $|\boldsymbol{P}-\boldsymbol{P}'| \gtrsim \sqrt{M/\beta}$, where $\sqrt{M/\beta}$ denotes the thermal momentum at temperature $T = 1/k_\mathrm{B}\beta$. Similarly, in position representation the coherence length should not be larger than the thermal de Broglie wavelength $\lambda_\mathrm{th} = \sqrt{2\pi\hbar^2\beta/M}$, which means $\langle \boldsymbol{X}|\rho|\boldsymbol{X}'\rangle \approx 0$ for $|\boldsymbol{X}-\boldsymbol{X}'| \gtrsim \lambda_\mathrm{th}$. We will see below that this allows one to linearize the Lindblad operator (6.3) with respect to the position and momentum operators.

At first, consider the gas particle momentum distribution (6.4) as it appears in the Lindblad operator (6.3),

$$\begin{aligned}\mu\left(\boldsymbol{k}_\perp + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\hat{\mathbf{P}}_\parallel\right) &= \mu(k_\perp, Q)\exp\left[-\frac{1}{p_\beta^2}\left(\left(\frac{m}{M}\right)^2\left|\hat{\mathbf{P}}_\parallel\right|^2 + \frac{m^2}{m_* M}\boldsymbol{Q}\cdot\hat{\mathbf{P}}_\parallel\right)\right] \\ &\approx \mu(k_\perp, Q)\exp\left[-\frac{m}{M p_\beta^2}\boldsymbol{Q}\cdot\hat{\mathbf{P}}_\parallel\right]. \end{aligned} \tag{6.14}$$

In the first line, I inserted the definition (6.11) for the Maxwell–Boltzmann distribution and in the second line I used that $m/M \ll 1$, which leads to the approximation $m_* \approx m$. The prefactor in the exponential in Eq. (6.14) is rewritten by noting that $p_\beta^2 = 2m/\beta$ and reads $\beta/2M$. Since the state is assumed to be close to thermal, the momentum transfer is of the order of the thermal momentum $p_\beta = \sqrt{2m/\beta}$, which leads to

$$\frac{\beta}{2M} Q\left|\boldsymbol{P}-\boldsymbol{P}'\right| \approx \sqrt{\frac{m}{M}}\sqrt{\frac{\beta}{2M}}\left|\boldsymbol{P}-\boldsymbol{P}'\right| \ll 1. \tag{6.15}$$

The estimation holds because the density matrix elements $\langle \boldsymbol{P}|\rho|\boldsymbol{P}'\rangle$ are assumed to be nonvanishing for $|\boldsymbol{P}-\boldsymbol{P}'| \lesssim \sqrt{M/\beta}$ only; furthermore $m/M \ll 1$ is used. In the end, this allows one to expand the exponential in Eq. (6.14) to first order resulting in the momentum distribution

$$\mu\left(\boldsymbol{k}_\perp + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\hat{\mathbf{P}}_\parallel\right) \approx \mu(k_\perp, Q)\left(1 - \frac{\beta}{2M}\boldsymbol{Q}\cdot\hat{\mathbf{P}}\right), \tag{6.16}$$

with the identity $\boldsymbol{Q}\cdot\hat{\mathbf{P}}_\parallel = \boldsymbol{Q}\cdot\hat{\mathbf{P}}$ used.

In a second step, the relative momenta (6.5) can be approximated by using again $m/M \ll 1$ and $m_* \approx m$,

$$\mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathsf{P}}\right) \approx \boldsymbol{k}_\perp. \tag{6.17}$$

In this regime, the isotropic scattering amplitude (6.9) reads

$$f\left(\mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathsf{P}}_\perp\right), Q\right) \approx f\left(k_\perp, Q\right). \tag{6.18}$$

Thirdly, the exponential in the Lindblad operator (6.10) that contains the position operator may be expanded to first order, too:

$$\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} \approx 1 - \frac{\mathrm{i}}{\hbar}\boldsymbol{Q}\cdot\hat{\mathbf{X}}. \tag{6.19}$$

This is permissible because it is assumed that $\langle \boldsymbol{X}|\rho|\boldsymbol{X}'\rangle$ is nonvanishing for $|\boldsymbol{X}-\boldsymbol{X}'| \lesssim \sqrt{2\pi\hbar^2\beta/M}$ only leading to

$$\frac{Q\,|\boldsymbol{X}-\boldsymbol{X}'|}{\hbar} \approx \sqrt{\frac{2m}{\hbar^2\beta}2\pi\hbar^2\frac{\beta}{M}} \ll 1. \tag{6.20}$$

Thus, putting together Eqs. (6.16), (6.18), and (6.19), the Lindblad operator (6.3) reads

$$\hat{\mathsf{L}}\left(\boldsymbol{k}_\perp, \boldsymbol{Q}\right) \approx \sqrt{\frac{n_{\mathrm{gas}}}{mQ}} f\left(k_\perp, Q\right) \sqrt{\mu\left(k_\perp, Q\right)} \left(1 + \frac{\mathrm{i}}{\hbar}\boldsymbol{Q}\cdot\hat{\mathbf{X}} - \frac{\beta}{4M}\boldsymbol{Q}\cdot\hat{\mathbf{P}}\right), \tag{6.21}$$

where I used that $m_* \approx m$ and that the term of second order in the operator dependence is much smaller than the other ones; it can therefore be neglected.

The dissipator (6.2) of the master equation can now be calculated by evaluating the integrals that occur therein. When writing down the different integrals explicitly, one recognizes that they simplify considerably, mainly due to the symmetry properties of the scattering amplitude and the gas momentum distribution. In particular, it is used that terms like $g\left(k_\perp, Q\right) Q_i$ vanish for arbitrary functions $g(k_\perp, Q)$, when integrated over $\boldsymbol{k}_\perp$ and $\boldsymbol{Q}$; see Appendix D.1 for the derivation of this relation. This fact shall be expressed by the shorthand notation $g\left(k_\perp, Q\right) Q_j \cong 0$, which means that "the left-hand side equals the right-hand side below the $\boldsymbol{k}_\perp$- and $\boldsymbol{Q}$- integrals", see Eq. (D.12). With the Lindblad operator (6.21), the integrand of the first summand of the dissipator (6.2) can then be written

$$\begin{aligned}\hat{\mathsf{L}}\left(\boldsymbol{k}_\perp, \boldsymbol{Q}\right) \rho \hat{\mathsf{L}}^\dagger\left(\boldsymbol{k}_\perp, \boldsymbol{Q}\right) &\cong \frac{n_{\mathrm{gas}}}{mQ} \left|f\left(k_\perp, Q\right)\right|^2 \mu\left(k_\perp, Q\right) \\ &\times \left\{\rho + \frac{Q^2}{3}\sum_{j=1}^{3}\left[\frac{1}{\hbar^2}\hat{\mathsf{X}}_j\rho\hat{\mathsf{X}}_j + \frac{\beta^2}{16M^2}\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_j - \frac{\mathrm{i}\beta}{4M\hbar}\left(\hat{\mathsf{X}}_j\rho\hat{\mathsf{P}}_j - \hat{\mathsf{P}}_j\rho\hat{\mathsf{X}}_j\right)\right]\right\},\end{aligned} \tag{6.22}$$

where I additionally used $g(k_\perp, Q)Q_jQ_k \cong \delta_{jk}g(k_\perp, Q)Q^2/3$ from Eq. (D.15). Treating the second summand analogously, gives

$$-\frac{1}{2}\left\{\rho, \hat{\mathsf{L}}^\dagger(\boldsymbol{k}_\perp, \boldsymbol{Q})\hat{\mathsf{L}}(\boldsymbol{k}_\perp, \boldsymbol{Q})\right\} \cong \frac{n_{\text{gas}}}{mQ}|f(k_\perp, Q)|^2\mu(k_\perp, Q) \times\left(-\frac{1}{2}\right)\left\{\rho, 1+\frac{Q^2}{3}\sum_{j=1}^{3}\left[\frac{1}{\hbar^2}\hat{\mathsf{X}}_j^2+\frac{\beta^2}{16M^2}\hat{\mathsf{P}}_j^2+\frac{\mathrm{i}\beta}{4M\hbar}\left(\hat{\mathsf{X}}_j\hat{\mathsf{P}}_j-\hat{\mathsf{P}}_j\hat{\mathsf{X}}_j\right)\right]\right\}. \quad (6.23)$$

From here, one directly derives the dissipator

$$\mathcal{D}\rho = -\gamma\sum_{j=1}^{3}\left\{\frac{M}{\hbar^2\beta}\left[\hat{\mathsf{X}}_j, \left[\hat{\mathsf{X}}_j, \rho\right]\right]+\frac{\beta}{16M}\left[\hat{\mathsf{P}}_j, \left[\hat{\mathsf{P}}_j, \rho\right]\right] +\frac{\mathrm{i}}{2\hbar}\left[\hat{\mathsf{X}}_j, \left\{\hat{\mathsf{P}}_j, \rho\right\}\right]+\frac{\mathrm{i}}{4\hbar}\left[\rho, \left\{\hat{\mathsf{X}}_j, \hat{\mathsf{P}}_j\right\}\right]\right\}, \quad (6.24)$$

where all integrals are hidden inside the *friction coefficient*

$$\gamma = \frac{\beta n_{\text{gas}}}{6Mm}\int \mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp Q\,|f(k_\perp, Q)|^2\,\mu(k_\perp, Q). \quad (6.25)$$

Moreover, the applied double commutators read

$$\begin{aligned}\left[\hat{\mathsf{A}}, \left[\hat{\mathsf{A}}, \rho\right]\right] &= \hat{\mathsf{A}}^2\rho+\rho\hat{\mathsf{A}}^2-2\hat{\mathsf{A}}\rho\hat{\mathsf{A}},\\ \left[\hat{\mathsf{A}}, \left\{\hat{\mathsf{B}}, \rho\right\}\right] &= \hat{\mathsf{A}}\hat{\mathsf{B}}\rho-\rho\hat{\mathsf{B}}\hat{\mathsf{A}}+\hat{\mathsf{A}}\rho\hat{\mathsf{B}}-\hat{\mathsf{B}}\rho\hat{\mathsf{A}}.\end{aligned} \quad (6.26)$$

The last summand in (6.24) has the structure of a Hamiltonian contribution and can be taken out of the dissipator and leads to the modified Hamilton operator,

$$\hat{\mathsf{H}} = \hat{\mathsf{H}}_0+\sum_{j=1}^{3}\frac{\gamma}{4}\left\{\hat{\mathsf{X}}_j, \hat{\mathsf{P}}_j\right\}. \quad (6.27)$$

This additional term represents a rescaled system energy due to the environmental coupling. Notice that the Hamiltonian correction $\hat{\mathsf{H}}_n$ of Eq. (6.6) does not contribute to the master equation, since the scattering amplitude is operator-independent.

Altogether, we arrive at the Lindblad master equation of QBM (3.56) that is build by the Hamiltonian (6.27) and the three Lindblad operators

$$\hat{\mathsf{L}}_j = \sqrt{\frac{M}{\hbar^2\beta}}\hat{\mathsf{X}}_j+\mathrm{i}\sqrt{\frac{\beta}{16M}}\hat{\mathsf{P}}_j. \quad (6.28)$$

Interestingly, the friction coefficient (6.25) has the same form as the one that is obtained via a classical derivation of Brownian motion starting from the classical linear Boltzmann equation [76, 77].

6.3. Expansion of the QLBE in the mass ratio

We have seen in the previous section that one arrives at the collisional decoherence limit of the QLBE by taking the test particle mass to infinity, or more precisely, by sending the mass ratio $\varepsilon \equiv m/M \to 0$. In that case, the $\hat{\mathbf{P}}$-dependence of the Lindblad operator vanishes, which leads to a non-dissipative master equation. It is desirable to go beyond the collisional decoherence limit and to derive a more realistic master equation, which allows finite mass ratios ε. This master equation will also be dissipative, since the Lindblad operator depends on both the position and momentum operator. Unlike the QBM master equation, where the Lindblad operator is linearized in its overall dependence on the operators $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$, in the following approximation scheme, one effectively linearizes the dependence on $\hat{\mathbf{P}}$ only.

To be specific, in what follows I will derive the aforementioned new master equation by Taylor expanding the Lindblad operator to first order in the mass ratio ε.

6.3.1. Expansion of the relevant terms

The Lindblad operator In the Lindblad operator (6.3) of the QLBE, one notices several occurences of the ratio $\varepsilon = m/M$; to deliver a most transparent expansion to first ε-order, I first consider each term separately and combine them to the Lindblad operator afterwards.

The prefactor in in the Lindblad operator (6.3), contains the term

$$\sqrt{\frac{m}{m_*^2}} = \frac{1+\varepsilon}{\sqrt{m}}, \tag{6.29}$$

which holds exactly. Secondly, inside the scattering amplitude there appear the relative momenta (6.5), which read

$$\mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathbf{P}}_\perp\right) = \boldsymbol{k}_\perp - \varepsilon\left(\boldsymbol{k}_\perp + \hat{\mathbf{P}}_\perp\right). \tag{6.30}$$

In a next step, the isotropic scattering amplitude (6.9) is Taylor expanded to first order in ε,

$$f\left(\left|\mathrm{rel}\left(\boldsymbol{k}_\perp, \hat{\mathbf{P}}_\perp\right)\right|, Q\right) \approx f\left(k_\perp, Q\right) - \varepsilon\left(k_\perp + \frac{\boldsymbol{k}_\perp \cdot \hat{\mathbf{P}}}{k_\perp}\right) f_{k_\perp}\left(k_\perp, Q\right), \tag{6.31}$$

where $f_{k_\perp}\left(k_\perp, Q\right) \equiv \partial f\left(k_\perp, Q\right)/\partial k_\perp$ and $\boldsymbol{k}_\perp \cdot \hat{\mathbf{P}}_\perp = \boldsymbol{k}_\perp \cdot \hat{\mathbf{P}}$ is used. The remaining term containing the momentum distribution of the gas particles (6.4) is also expanded and gives

$$\begin{aligned}\sqrt{\mu\left(\boldsymbol{k}_\perp + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\hat{\mathbf{P}}_\parallel\right)} &= \sqrt{\mu\left(\boldsymbol{k}_\perp + \frac{\boldsymbol{Q}}{2} + \varepsilon\left(\frac{\boldsymbol{Q}}{2} + \hat{\mathbf{P}}_\parallel\right)\right)} \\ &\approx \sqrt{\mu\left(k_\perp, Q\right)}\left(1 - \frac{\varepsilon}{2p_\beta^2}\left(\frac{Q^2}{2} + \boldsymbol{Q}\cdot\hat{\mathbf{P}}\right)\right),\end{aligned} \tag{6.32}$$

where I used $m/m_* = 1+\varepsilon$ and the definition (6.11) of $\mu(k_\perp, Q)$.

Finally, the Lindblad operator (6.3) can be written down by putting together Eqs. (6.29)-(6.32) and keeping terms up to first order in ε only:

$$\hat{\mathsf{L}}\left(\boldsymbol{k}_\perp, \boldsymbol{Q}\right) \approx \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{x}}/\hbar}\sqrt{\frac{n_{\mathrm{gas}}}{mQ}\mu\left(k_\perp, Q\right)}\Bigg[\left(1+\varepsilon\right)f\left(k_\perp, Q\right) - \varepsilon f_{k_\perp}\left(k_\perp, Q\right)\left(k_\perp + \frac{\boldsymbol{k}_\perp\cdot\hat{\mathbf{P}}}{k_\perp}\right) - \frac{\varepsilon}{2p_\beta^2}f\left(k_\perp, Q\right)\left(\frac{Q^2}{2} + \boldsymbol{Q}\cdot\hat{\mathbf{P}}\right)\Bigg]. \quad (6.33)$$

It is easily observed that the Lindblad operator of collisional decoherence (6.10) is recovered in the limit $\varepsilon \to 0$.

For what follows, the Lindblad operator (6.33) is brought into a more convenient form by using the abbreviations

$$\begin{aligned}\mathcal{A} &= \frac{n_{\mathrm{gas}}}{mQ}\mu\left(k_\perp, Q\right),\\ \lambda_0 &= f + \varepsilon\left(f\left(1 - \frac{Q^2}{4p_\beta^2}\right) - f_{k_\perp}k_\perp\right),\\ \boldsymbol{\lambda}_1 &= \varepsilon\left(f\frac{\boldsymbol{Q}}{2p_\beta^2} + f_{k_\perp}\frac{\boldsymbol{k}_\perp}{k_\perp}\right),\end{aligned} \quad (6.34)$$

as well as $f \equiv f\left(k_\perp, Q\right)$ and $f_{k_\perp} \equiv f_{k_\perp}\left(k_\perp, Q\right)$. The Lindblad operator then reads

$$\hat{\mathsf{L}} \equiv \hat{\mathsf{L}}\left(\boldsymbol{k}_\perp, \boldsymbol{Q}\right) = \sqrt{\mathcal{A}}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{x}}/\hbar}\left(\lambda_0 - \boldsymbol{\lambda}_1\cdot\hat{\mathbf{P}}\right). \quad (6.35)$$

The Hamiltonian correction The Hamiltonian correction (6.6) does not contribute to the master equation, when expanded to first order in ε. To see this, one needs to Taylor expand the scattering amplitude that appears therein. Similar to the preceding derivation, for isotropic scattering processes and written in the variables $\boldsymbol{p}_\perp$ and $\boldsymbol{Q}$, see Eq. (6.9), one gets

$$f\left(\left|\mathrm{rel}\left(\boldsymbol{p}, \hat{\mathbf{P}}\right)\right|, 0\right) \approx f\left(p, 0\right) - \varepsilon\left(p + \frac{\boldsymbol{p}\cdot\hat{\mathbf{P}}}{p}\right)f_p\left(p, 0\right). \quad (6.36)$$

With the above approximation of the scattering amplitude, the Hamiltonian correction (6.6), when written to first order in ε, attains the form

$$\hat{\mathsf{H}}_{\mathrm{n}} \approx -2\pi\hbar^2\frac{n_{\mathrm{gas}}}{m}\int \mathrm{d}\boldsymbol{p}\mu(p, 0)\left[\mathrm{Re}\left\{f\left(p, 0\right)\right\}\left(1+\varepsilon\right) - \varepsilon\left(p + \frac{\boldsymbol{p}\cdot\hat{\mathbf{P}}}{p}\right)\mathrm{Re}\left\{f_p\left(p, 0\right)\right\}\right], \quad (6.37)$$

where I used $1/m_* = \left(1+\varepsilon\right)/m$. Moreover, I substituted Eq. (6.11) for the momentum distribution of the gas particles $\mu(\boldsymbol{p})$ to take account of its isotropy.

Since $\hat{\mathsf{H}}_\mathrm{n}$ appears in the master equation (6.1) inside the commutator only, it is just the operator-dependent term that contributes. In this remaining relevant term in Eq. (6.37), one may split the integration over $\boldsymbol{p}$ into the radial and the angular part over p and $\boldsymbol{\Omega}$, respectively. As one easily verifies, the latter integral vanishes:

$$\int \mathrm{d}\boldsymbol{\Omega}\boldsymbol{p}\cdot\hat{\mathbf{P}} = 0, \tag{6.38}$$

which leads to a vanishing contribution in the whole. In conclusion, up to first order in ε, there is *no contribution* of the Hamiltonian correction $\hat{\mathsf{H}}_\mathrm{n}$ to the master equation.

6.3.2. Derivation of the master equation

The dissipator (6.2) of the QLBE consists of several terms; let us start by considering the first one. Upon inserting the Lindblad operator (6.35), one obtains for the integrand of the first term of the dissipator (6.2),

$$\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger = \mathcal{A}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\left[|\lambda_0|^2\,\rho - \lambda_0\boldsymbol{\lambda}_1^*\cdot\rho\hat{\mathbf{P}} - \lambda_0^*\boldsymbol{\lambda}_1\cdot\hat{\mathbf{P}}\rho + \hat{\mathbf{P}}\cdot(\boldsymbol{\lambda}_1\otimes\boldsymbol{\lambda}_1^*)\cdot\rho\hat{\mathbf{P}}\right]\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}. \tag{6.39}$$

In anticipation of the dynamics of the phase space expectations and variances of the master equation, I relate the four terms in square brackets in Eq. (6.39) to specific constants describing, for instance, diffusion and friction. The first summand corresponds to the momentum diffusion constant D_p and I define it by introducing an appropriate integral kernel D_p^K,

$$\begin{aligned} D_p &= \int \mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp D_p^\mathrm{K}, \\ D_p^\mathrm{K} &= \mathcal{A}\frac{1}{3}Q^2\,|\lambda_0|^2 = \mathcal{A}\frac{1}{3}Q^2\left[|f|^2 + 2\varepsilon\left(|f|^2\left(1-\frac{Q^2}{4p_\beta^2}\right) - \frac{1}{2}\,|f|_{k_\perp}^2\,k_\perp\right)\right. \\ &\qquad \left. + \varepsilon^2\left(|f|^2\left(1-\frac{Q^2}{4p_\beta^2}\right)^2 - |f|_{k_\perp}^2\,k_\perp\left(1-\frac{Q^2}{4p_\beta^2}\right) + |f_{k_\perp}|^2\,k_\perp^2\right)\right], \end{aligned} \tag{6.40}$$

with the shorthand notation $|f|_{k_\perp}^2 = 2\mathrm{Re}\left\{f f_{k_\perp}^*\right\}$. Here and in the following, the superscript "K" denotes the integral kernel, which yields the corresponding constant when integrated over $\boldsymbol{Q}$ and $\boldsymbol{k}_\perp$.

The second and third summands in the square brackets in Eq. (6.39) may be rewritten into the form

$$-\frac{\varepsilon}{2p_\beta^2}\mathrm{Re}\left\{\lambda_0 f^*\right\}\left\{\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right\} + \mathrm{i}\frac{\varepsilon}{2p_\beta^2}\mathrm{Im}\left\{\lambda_0 f^*\right\}\left[\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right], \tag{6.41}$$

where I used that, according to Eq. (D.10), the terms including the vector $\boldsymbol{k}_\perp$ vanish. The first term in Eq. (6.41) gives rise to the friction constant η and its associated integral

kernel,

$$\begin{aligned}\eta &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \eta^{\mathrm{K}},\\ \eta^{\mathrm{K}} &= \frac{\mathcal{A}}{3}\frac{\varepsilon}{2p_\beta^2} 2\mathrm{Re}\left\{\lambda_0 f^*\right\} Q^2 = \mathcal{A}\frac{\varepsilon}{3}\frac{Q^2}{p_\beta^2}\left[|f|^2 + \varepsilon\left(|f|^2\left(1-\frac{Q^2}{4p_\beta^2}\right) - \frac{1}{2}\left|f\right|^2_{k_\perp} k_\perp\right)\right].\end{aligned} \tag{6.42}$$

The second term leads to the introduction of the covariance diffusion constant D_{xp},

$$\begin{aligned}D_{xp} &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp D_{xp}^{\mathrm{K}},\\ D_{xp}^{\mathrm{K}} &= \frac{\mathcal{A}}{3}\frac{\hbar\varepsilon}{2p_\beta^2}\mathrm{Im}\left\{\lambda_0 f^*\right\} Q^2 = \mathcal{A}\frac{\hbar\varepsilon^2}{6}\mathrm{Im}\left\{f f^*_{k_\perp}\right\} k_\perp \frac{Q^2}{p_\beta^2}.\end{aligned} \tag{6.43}$$

Finally, the fourth summand in Eq. (6.39) can also be simplified by exploiting the symmetry properties of the integrand. Notice that most of the integrals that appear in the following can be reduced in complexity due to their symmetry properties. I already took advantage of this fact in the derivation of the QBM master equation, cf. Eqs. (6.22) and (6.23), as well as in Eq. (6.41). Specifically, I now use for arbitrary functions $g(k_\perp, \boldsymbol{Q})$ the relations $g(k_\perp, \boldsymbol{Q})\boldsymbol{k}_\perp \cong 0$ and

$$g\left(k_\perp, \boldsymbol{Q}\right)\frac{\boldsymbol{k}_\perp \otimes \boldsymbol{k}_\perp}{k_\perp^2} \cong \frac{1}{2} g\left(k_\perp, \boldsymbol{Q}\right)\left(\mathbb{1} - \frac{\boldsymbol{Q}\otimes\boldsymbol{Q}}{Q^2}\right), \tag{6.44}$$

which are derived in Eqs. (D.10) and (D.11) in Appendix D.1. Remember that the "$\cong$"-sign denotes equality of the integrands when integrated over the momenta $\boldsymbol{Q}$ and $\boldsymbol{k}_\perp$. For the fourth summand in the square brackets in Eq. (6.39) I then get

$$\hat{\mathbf{P}}\cdot\left(\boldsymbol{\lambda}_1 \otimes \boldsymbol{\lambda}_1^*\right)\cdot\rho\hat{\mathbf{P}} \cong \varepsilon^2\hat{\mathbf{P}}\cdot\left(\left(\frac{|f|^2}{4p_\beta^4} - \frac{|f_{k_\perp}|^2}{2Q^2}\right)\boldsymbol{Q}\otimes\boldsymbol{Q} + \frac{|f_{k_\perp}|^2}{2}\mathbb{1}\right)\cdot\rho\hat{\mathbf{P}}, \tag{6.45}$$

which motivates the introduction of the position diffusion constant

$$\begin{aligned}D_x &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp D_x^{\mathrm{K}},\\ D_x^{\mathrm{K}} &= \mathcal{A}\frac{\hbar^2}{3}\left|\boldsymbol{\lambda}_1\right|^2 = \mathcal{A}\frac{\hbar^2\varepsilon^2}{3}\left(|f|^2\frac{Q^2}{4p_\beta^4} + |f_{k_\perp}|^2\right),\end{aligned} \tag{6.46}$$

and the energy correction

$$\begin{aligned}\nu &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \nu^{\mathrm{K}},\\ \nu^{\mathrm{K}} &= \mathcal{A}\frac{\varepsilon^2}{6} Q^2 \left|f_{k_\perp}\right|^2.\end{aligned} \tag{6.47}$$

Altogether, the first dissipative part (6.39) reads

$$\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger \cong \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\frac{3}{Q^2}\Bigg[D_p^{\mathrm{K}}\rho - \frac{\eta^{\mathrm{K}}}{2}\left\{\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right\} + \mathrm{i}D_{xp}^{\mathrm{K}}\left[\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right] \\ + \left(\frac{D_x^{\mathrm{K}}}{\hbar^2} - \frac{3\nu^{\mathrm{K}}}{Q^2}\right)\sum_{j,k=1}^{3} Q_jQ_k\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_k + \nu^{\mathrm{K}}\sum_{j=1}^{3}\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_j\Bigg]\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}. \quad (6.48)$$

Coming to the second term of the dissipator (6.2), one observes that it involves the product $\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}$, which leads to the dissappearance of its position operator dependence; therefore, the $\boldsymbol{Q}$-dependence of the integrand turns much simpler. One arrives at

$$-\frac{1}{2}\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\} \cong -\frac{3D_p^{\mathrm{K}}}{Q^2}\rho - \frac{D_x^{\mathrm{K}}}{2\hbar^2}\left\{\hat{\mathbf{P}}^2,\rho\right\}, \quad (6.49)$$

where the integrand is simplified by using the two previous relations affecting the $\boldsymbol{k}_\perp$-integrals as well as $g(k_\perp,Q)\boldsymbol{Q} \cong 0$ and $g(k_\perp,Q)Q_j^2 \cong g(k_\perp,Q)Q^2/3$, see Eqs. (D.10), (D.11), (D.13), and (D.15), respectively.

6.3.3. The master equation of dissipative collisional decoherence

With the above calculations and definitions, it is straightforward to write down the whole master equation by substituting the dissipator terms (6.48) and (6.49) into Eqs. (6.1) and (6.2). One arrives at

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}_0,\rho\right] + \int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\frac{3}{Q^2}\Bigg[D_p^{\mathrm{K}}\left(\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\rho\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} - \rho\right) \\ + \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\left(-\frac{\eta^{\mathrm{K}}}{2}\left\{\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right\} + \mathrm{i}D_{xp}^{\mathrm{K}}\left[\boldsymbol{Q}\cdot\hat{\mathbf{P}},\rho\right]\right)\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} \\ + \frac{D_x^{\mathrm{K}}}{\hbar^2}\left(\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\sum_{j,k=1}^{3}Q_jQ_k\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_k\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} - \frac{Q^2}{6}\left\{\hat{\mathbf{P}}^2,\rho\right\}\right) \\ + \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\nu^{\mathrm{K}}\left(\sum_{j=1}^{3}\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_j - \frac{3}{Q^2}\sum_{j,k=1}^{3}Q_jQ_k\hat{\mathsf{P}}_j\rho\hat{\mathsf{P}}_k\right)\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\Bigg], \quad (6.50)$$

I call this master equation the *dissipative collisional decoherence master equation.*

In the following, I derive equations of motion for the position and momentum expectations as well as for the corresponding variances; they reveal a dissipative and diffusive behavior of the master equation. After that, I examine its decoherence properties, which turn out to be very similar to those of collisional decoherence; finally, I discuss aspects regarding the induced pointer states.

As we will see, the D_p^{K}-term in the master equation (6.50) is responsible for the main effect of the decoherence properties and also produces the momentum diffusion

constant, which appears in the equation of motion of the momentum variance. The two summands in the second line of (6.50) give rise to the friction constant and the covariance diffusion constant. In the same way, the term containing D_x^{K} in the third line yields the position diffusion and the fourth line gives rise to an energy correction of the momentum variance. Note that all integral kernels depend on Q and $k_\perp$, although this is not written explicitly.

6.4. Expectation values of the master equation

In this section, I first derive the equations of motion for the position and momentum expectation values as well as those of the position and momentum variance and the covariance. Second, the set of differential equations is solved and discussed.

6.4.1. Equations of motion

In a first step, I derive the differential equations of the position and momentum expectations as well as of the variances, which show friction and diffusion effects. In general, the equation of motion for an arbitrary (time-independent) hermitian operator $\hat{\mathbf{A}}$ evolving according to the master equation (6.50) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{\boldsymbol{A}} = \mathrm{Tr}\left\{\frac{\mathrm{d}}{\mathrm{d}t}\rho\hat{\mathbf{A}}\right\} = \mathrm{Tr}\left\{\left[\frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}_0,\rho\right] + \int \mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\left(\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger - \frac{1}{2}\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\right)\right]\hat{\mathbf{A}}\right\}, \tag{6.51}$$

with the two dissipative terms defined in Eqs. (6.48) and (6.49). The free Hamiltonian has the form $\hat{\mathsf{H}}_0 = \hat{\mathbf{P}}^2/2M$.

Position expectation The contribution of the Hamiltonian term is straightforwardly calculated by using the cyclic invariance of the trace. One gets

$$\frac{1}{2\mathrm{i}\hbar M}\mathrm{Tr}\left\{\rho\left[\hat{\mathbf{X}},\hat{\mathbf{P}}^2\right]\right\} = \frac{\overline{\boldsymbol{P}}}{M}. \tag{6.52}$$

In the calculation of the contribution of the first dissipative term with integrand $\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger$ from Eq. (6.48), one remarks that the position operator dependence of the Lindblad operator dissappears because $\exp\left(\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar\right)$ and $\hat{\mathbf{X}}$ commute and due to the cyclic invariance of the trace. Then, one uses relations (D.13) and (D.15) to see that all terms with an odd power of Q_i vanish, which affects the terms with η^{K}, D_{xp}^{K}, and ν^{K}. Thus, one gets as first dissipative contribution from Eq. (6.48),

$$\mathrm{Tr}\left\{\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger\hat{\mathbf{X}}\right\} \cong \frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\boldsymbol{X}} + \frac{D_x^{\mathrm{K}}}{\hbar^2}\sum_{j=1}^{3}\mathrm{Tr}\left\{\rho\hat{\mathsf{P}}_j\hat{\mathbf{X}}\hat{\mathsf{P}}_j\right\}. \tag{6.53}$$

The second dissipative term (6.49) gives

$$-\frac{1}{2}\mathrm{Tr}\left\{\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\hat{\mathbf{X}}\right\}\cong-\frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\boldsymbol{X}}-\frac{D_x^{\mathrm{K}}}{2\hbar^2}\sum_{j=1}^{3}\mathrm{Tr}\left\{\rho\left(\hat{\mathsf{P}}_j^2\hat{\mathbf{X}}+\hat{\mathbf{X}}\hat{\mathsf{P}}_j^2\right)\right\}. \tag{6.54}$$

These two contributions sum up to zero, which easily follows from $2\hat{\mathsf{P}}_j\hat{\mathsf{X}}_i\hat{\mathsf{P}}_j-\hat{\mathsf{P}}_j^2\hat{\mathsf{X}}_i-\hat{\mathsf{X}}_i\hat{\mathsf{P}}_j^2=\left[\hat{\mathsf{P}}_j,\left[\hat{\mathsf{X}}_i,\hat{\mathsf{P}}_j\right]\right]=0$. Altogether, one arrives at

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{\boldsymbol{X}}=\frac{\overline{\boldsymbol{P}}}{M}. \tag{6.55}$$

Momentum expectation For the momentum expectation, the Hamiltonian term gives no contribution because only commuting momentum operators are involved. In contrast to the previous derivation, the dependence of the first dissipative term on the position operator does not vanish in this case. However, it can be treated by exploiting the cyclic invariance of the trace again. Using the commutator

$$\left[\hat{\mathbf{P}},\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right]=\boldsymbol{Q}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}, \tag{6.56}$$

one derives

$$\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}=\hat{\mathbf{P}}+\boldsymbol{Q}. \tag{6.57}$$

Along with the symmetries of the $\boldsymbol{Q}$-integration (for instance, terms of odd power in Q_i vanish), one then obtains for the first dissipative term (6.48)

$$\mathrm{Tr}\left\{\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger\hat{\mathbf{P}}\right\}\cong\frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\boldsymbol{P}}-\eta^{\mathrm{K}}\overline{\boldsymbol{P}}+\frac{D_x^{\mathrm{K}}}{\hbar^2}\overline{\boldsymbol{P}^2\boldsymbol{P}}. \tag{6.58}$$

Similarly, the second dissipative term (6.49) yields

$$-\frac{1}{2}\mathrm{Tr}\left\{\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\hat{\mathbf{P}}\right\}\cong-\frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\boldsymbol{P}}-\frac{D_x^{\mathrm{K}}}{\hbar^2}\overline{\boldsymbol{P}^2\boldsymbol{P}}. \tag{6.59}$$

Taking both contributions together, the differential equation for the momentum reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{\boldsymbol{P}}=-\eta\overline{\boldsymbol{P}}, \tag{6.60}$$

where the friction constant is defined in Eqs. (6.42).

Position variance To calculate the equation of motion of the position variance, one derives a differential equation for the second moment of the position operator $\hat{\mathsf{X}}_i$. Afterwards the equation of motion for the variance is calculated via the relation $\mathrm{d}V_{x,i}/\mathrm{d}t=\mathrm{d}\overline{X_i^2}/\mathrm{d}t-2\overline{X}_i\mathrm{d}\overline{X}_i/\mathrm{d}t$. As in the calculation of the first position moment, the Hamiltonian contribution boils down to the calculation of a commutator,

$$\frac{1}{2\mathrm{i}\hbar M}\mathrm{Tr}\left\{\rho\left[\hat{\mathsf{X}}_i^2,\hat{\mathbf{P}}^2\right]\right\}=\frac{\overline{\{X_i,P_i\}}}{M}. \tag{6.61}$$

The dissipative contributions are obtained analogously to the calculation of the first position moment, cf. Eqs. (6.53) and (6.54). One arrives at

$$\mathrm{Tr}\left\{\left(\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger - \frac{1}{2}\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\right)\hat{\mathsf{X}}_i^2\right\} \cong \frac{D_x^{\mathrm{K}}}{2\hbar^2}\sum_{j=1}^{3}\mathrm{Tr}\left\{\rho\left(2\hat{\mathsf{P}}_j\hat{\mathsf{X}}_i^2\hat{\mathsf{P}}_j - \hat{\mathsf{P}}_j^2\hat{\mathsf{X}}_i^2 - \hat{\mathsf{X}}_i^2\hat{\mathsf{P}}_j^2\right)\right\} = D_x^{\mathrm{K}}, \tag{6.62}$$

with $2\hat{\mathsf{P}}_j\hat{\mathsf{X}}_i^2\hat{\mathsf{P}}_j - \hat{\mathsf{P}}_j^2\hat{\mathsf{X}}_i^2 - \hat{\mathsf{X}}_i^2\hat{\mathsf{P}}_j^2 = \left[\hat{\mathsf{P}}_j,\left[\hat{\mathsf{X}}_i^2,\hat{\mathsf{P}}_j\right]\right] = 2\hbar^2\delta_{ij}$.

For the variance, one then finds

$$\frac{\mathrm{d}}{\mathrm{d}t}V_{x,i} = \frac{C_{xp,i}}{M} + D_x, \tag{6.63}$$

with the covariance $C_{xp,i}$ and the position diffusion constant, which is introduced in Eqs. (6.46).

Momentum variance The equation of motion of the momentum variance is calculated by deriving the second moment of $\hat{\mathsf{P}}_i$ first. Similar as for the momentum expectation, the Hamiltonian contribution vanishes and one needs to care about the two dissipative terms only. To account for the position operator dependence in the $\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger$-term, one uses

$$\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathsf{P}}_i^2\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} = \left(\hat{\mathsf{P}}_i + Q_i\right)^2 = \hat{\mathsf{P}}_i^2 + 2Q_i\hat{\mathsf{P}}_i + Q_i^2, \tag{6.64}$$

which is derived with the help of Eq. (6.57). The first dissipative term (6.48), which one evaluates with the above relation and with the help of Appendix D.1, reads

$$\begin{aligned}\mathrm{Tr}\left\{\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger\hat{\mathsf{P}}_i^2\right\} \cong D_p^{\mathrm{K}}\left(\frac{3}{Q^2}\overline{P_i^2}+1\right) - 2\eta^{\mathrm{K}}\overline{P_i^2} + \frac{D_x^{\mathrm{K}}}{\hbar^2}\overline{\boldsymbol{P}^2P_i^2} + \nu^{\mathrm{K}}\overline{\boldsymbol{P}^2} \\ + \frac{3}{Q^2}\left(\frac{D_x^{\mathrm{K}}}{\hbar^2} - \frac{3\nu^{\mathrm{K}}}{Q^2}\right)\sum_{j=1}^{3}Q_i^2Q_j^2\overline{P_j^2}.\end{aligned} \tag{6.65}$$

For the second dissipative contribution (6.49), one derives

$$-\frac{1}{2}\mathrm{Tr}\left\{\left\{\rho,\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\hat{\mathsf{P}}_i^2\right\} \cong -\frac{3D_p^{\mathrm{K}}}{Q^2}\overline{P_i^2} - \frac{D_x^{\mathrm{K}}}{\hbar^2}\overline{\boldsymbol{P}^2P_i^2}. \tag{6.66}$$

Together with the equation of motion of the momentum expectation (6.60), the differential equation for the momentum variance is infered,

$$\frac{\mathrm{d}}{\mathrm{d}t}V_{p,i} = D_p - 2\eta V_{p,i} + \nu\overline{\boldsymbol{P}^2} + \int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\frac{3}{Q^2}\left(\frac{D_x^{\mathrm{K}}}{\hbar^2} - \frac{3\nu^{\mathrm{K}}}{Q^2}\right)\sum_{j=1}^{3}Q_i^2Q_j^2\overline{P_j^2}, \tag{6.67}$$

where D_p, η, ν, and D_x are defined in Eqs. (6.40), (6.42), (6.46), and (6.47).

Covariance The covariance $C_{xp,i} = \overline{\{X_i, P_i\}} - 2\overline{X}_i\overline{P}_i$ is treated by first calculating the equation of motion of the anticommutator term. The Hamiltonian contribution reads

$$\frac{1}{2\mathrm{i}\hbar M}\mathrm{Tr}\left\{\rho\left(2\left[\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\hat{\mathbf{P}}^2\right] - \left\{\hat{\mathbf{P}}^2, \left[\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right]\right\}\right)\right\} = 2\frac{\overline{P_i^2}}{M}. \tag{6.68}$$

In the dissipative terms, the exponential that contains the position operator is dealt with, as before, by shifting the momentum operators by Q_i, in particular,

$$\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\left\{\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right\}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar} = \left\{\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right\} + 2Q_i\hat{\mathsf{X}}_i, \tag{6.69}$$

which is derived with the help of Eq. (6.57). It is then straightforward to calculate the first dissipative contribution (6.48),

$$\mathrm{Tr}\left\{\hat{\mathsf{L}}\rho\hat{\mathsf{L}}^\dagger\left\{\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right\}\right\} \cong \frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\{X_i, P_i\}} - \eta^{\mathrm{K}}\overline{\{X_i, P_i\}} + D_{xp}^{\mathrm{K}} + \frac{D_x^{\mathrm{K}}}{\hbar^2}\sum_{j=1}^{3}\overline{P_j\{X_i, P_i\}P_j}. \tag{6.70}$$

The second contribution (6.49) gives

$$-\frac{1}{2}\mathrm{Tr}\left\{\left\{\rho, \hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right\}\left\{\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right\}\right\} \cong -\frac{3D_p^{\mathrm{K}}}{Q^2}\overline{\{X_i, P_i\}} - \frac{D_x^{\mathrm{K}}}{2\hbar^2}\left(\overline{\boldsymbol{P}^2\{X_i, P_i\}} + \overline{\{X_i, P_i\}\boldsymbol{P}^2}\right). \tag{6.71}$$

Taking both terms together, the vanishing double commutator $\left[\hat{\mathsf{P}}_j, \left[\left\{\hat{\mathsf{X}}_i, \hat{\mathsf{P}}_i\right\}, \hat{\mathsf{P}}_j\right]\right] = 0$ leads to a cancellation of the summands involving D_x^{K}.

Finally, together with the two differential equations for the position and momentum expectations, Eqs. (6.55) and (6.60), one arrives at the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}C_{xp,i} = \frac{2}{M}V_{p,i} - \eta C_{xp,i} + D_{xp}, \tag{6.72}$$

where η and D_{xp} are defined in Eqs. (6.42) and (6.43).

Mean energy The expectation value of the kinetic energy reads $\overline{E} = \overline{\boldsymbol{P}^2}/2M$; its equation of motion is readily derived from the one of the momentum variance Eq. (6.67):

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{E} = \frac{1}{2M}\left(\sum_{i=1}^{3}\frac{\mathrm{d}}{\mathrm{d}t}V_{p,i} + 2\overline{\boldsymbol{P}}\cdot\frac{\mathrm{d}}{\mathrm{d}t}\overline{\boldsymbol{P}}\right) = \frac{3D_p}{2M} - \left(2\eta - \int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\frac{D_x^{\mathrm{K}}Q^2}{\hbar^2}\right)\overline{E}. \tag{6.73}$$

6.4.2. Solutions of the equations of motion

Position and momentum expectation The equations of motion for the first moments, Eqs. (6.55) and (6.60), are already known from the previous chapters and they describe an exponentially damped momentum. For the initial values $\boldsymbol{X}_0$ and $\boldsymbol{P}_0$ their solutions read

$$\begin{aligned}\overline{\boldsymbol{X}}(t) &= \boldsymbol{X}_0 + \frac{\boldsymbol{P}_0}{M\eta}\left(1 - \mathrm{e}^{-\eta t}\right),\\ \overline{\boldsymbol{P}}(t) &= \boldsymbol{P}_0\mathrm{e}^{-\eta t}.\end{aligned} \tag{6.74}$$

Mean energy The differential equations for the variances, the covariance, and the energy form a closed set, which is solved successively by starting with the energy. From Eq. (6.73), the solution is readily obtained,

$$\overline{E}(t) = (E_0 - E_\infty)\,\mathrm{e}^{-\alpha t} + E_\infty, \tag{6.75}$$

with $\alpha = 2\eta - \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp D_x^{\mathrm{K}} Q^2/\hbar^2$, the inital energy E_0, and the asymptotic energy $E_\infty = 3D_p/2M\alpha$ for $t \to \infty$. To vanishing order in the parameter ε, one retrieves for E_∞ the thermal energy $3k_{\mathrm{B}}T/2$ expected by the equipartition theorem. If one includes the terms up to first order in ε, one gets

$$\begin{aligned} E_\infty = {} & \frac{3}{2} k_{\mathrm{B}} T\,(1+\varepsilon) - \frac{3}{32m}\frac{A_4}{A_2}\varepsilon \\ & + \frac{3}{2} k_{\mathrm{B}} T \frac{1}{A_2} \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mathcal{A} \left(m k_{\mathrm{B}} T\,|f_{k_\perp}|^2\, Q^2 - \frac{1}{2}\,|f|^2\, k_\perp Q^2 \right) \varepsilon + \mathcal{O}\left(\varepsilon^2\right), \end{aligned} \tag{6.76}$$

with $A_n = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mathcal{A}\,|f|^2\, Q^n$. This value differs from the equipartition value because the ε-dependence is truncated in contrast to the full QLBE.

Momentum variance In order to solve the differential equation (6.67) of the momentum variance, it is helpful to bring it into the form

$$\frac{\mathrm{d}}{\mathrm{d}t} V_{p,i} = D_p - (2\eta + \mu_{\mathrm{OD}} - \mu_{\mathrm{D}})\, V_{p,i} + 2M\,(\nu + \mu_{\mathrm{OD}})\,\overline{E}(t) - (\mu_{\mathrm{OD}} - \mu_{\mathrm{D}})\,\overline{P}_i^2(t), \tag{6.77}$$

where μ_{D} and μ_{OD} are the diagonal and off-diagonal elements of the matrix

$$\begin{aligned} \mu_{jk} &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mu_{jk}^{\mathrm{K}}, \\ \mu_{jk}^{\mathrm{K}} &= \frac{3}{Q^2}\left(\frac{D_x^{\mathrm{K}}}{\hbar^2} - \frac{3\nu^{\mathrm{K}}}{Q^2} \right) Q_j^2 Q_k^2 = \mathcal{A}\varepsilon^2 \left(\frac{|f|^2}{4p_\beta^4} - \frac{|f_{k_\perp}|^2}{2Q^2} \right) Q_j^2 Q_k^2. \end{aligned} \tag{6.78}$$

Due to the symmetry of the integral kernel, μ_{jk} has only two different elements, the diagonal elements $\mu_{\mathrm{D}} \equiv \mu_{jj}$ and the off-diagonal elements $\mu_{\mathrm{OD}} \equiv \mu_{jk}$ for $j \neq k$.

With the solutions for the momentum expectation and the energy, Eqs. (6.74) and (6.75), it is straightforward to solve Eq. (6.77), which gives after some algebra,

$$V_{p,i}(t) = 2M \left(E_{0,i} - \frac{E_0}{3} \right) \mathrm{e}^{-(2\eta + \mu_{\mathrm{OD}} - \mu_{\mathrm{D}})t} + \frac{2M}{3}\overline{E}(t) - \overline{P}_i^2(t), \tag{6.79}$$

with $E_{0,i}$ the initial energy in the cartesian component i. In the derivation of Eq. (6.79), I use the relation

$$3\nu^{\mathrm{K}} + 2\mu_{\mathrm{OD}}^{\mathrm{K}} + \mu_{\mathrm{D}}^{\mathrm{K}} = \frac{D_x^{\mathrm{K}}}{\hbar^2} Q^2, \tag{6.80}$$

which follows from the definitions (6.46), (6.47), and (6.78) of the appropriate kernels. In general, $V_{p,i}(t)$ is different for all cartesian components, however, for large times, the momentum variance (6.79) approaches the asymptotic value $2ME_\infty/3 = D_p/\alpha$, which is the same for all i.

Covariance and position variance Having the momentum variance at hand, one can now derive the covariance via Eq. (6.72) and subsequently the position variance via Eq. (6.63). A direct calculation leads to the solutions

$$C_{xp,i}(t) = C_{xp,0,i}\mathrm{e}^{-\eta t} - 2\left(\overline{X}_i(t) - X_{0,i}\right)\overline{P}_i(t) + \left(\frac{4}{3}E_\infty + D_{xp}\right)\frac{1-\mathrm{e}^{-\eta t}}{\eta} + 4\left(E_{0,i} - \frac{E_0}{3}\right)\mathrm{e}^{-\eta t}\frac{1-\mathrm{e}^{-(\eta+\mu_{\mathrm{OD}}-\mu_{\mathrm{D}})t}}{\eta+\mu_{\mathrm{OD}}-\mu_{\mathrm{D}}} + \frac{4}{3}\left(\overline{E}(t) - E_\infty\right)\frac{1-\mathrm{e}^{-(\eta-\alpha)t}}{\eta-\alpha}, \quad (6.81)$$

and

$$V_{x,i}(t) = V_{x,0,i} - \left(\overline{X}_i(t) - X_{0,i}\right)^2 + \left(\frac{2D_p}{M^2\eta\alpha} + \frac{D_{xp}}{M\eta} + D_x\right)t + \left(C_{xp,0,i} - \frac{2D_p}{\eta\alpha} - \frac{D_{xp}}{\eta}\right)\frac{1-\mathrm{e}^{-\eta t}}{M\eta} - \frac{4\left(E_0 - E_\infty\right)}{3M\left(\eta-\alpha\right)}\left(\frac{1-\mathrm{e}^{-\eta t}}{\eta} - \frac{1-\mathrm{e}^{-\alpha t}}{\alpha}\right) + \frac{4\left(E_{0,i} - E_0/3\right)}{M\left(\eta+\mu_{\mathrm{OD}}-\mu_{\mathrm{D}}\right)}\left(\frac{1-\mathrm{e}^{-\eta t}}{\eta} - \frac{1-\mathrm{e}^{-(2\eta+\mu_{\mathrm{OD}}-\mu_{\mathrm{D}})t}}{2\eta+\mu_{\mathrm{OD}}-\mu_{\mathrm{D}}}\right), \quad (6.82)$$

where $C_{xp,o,i}$ and $V_{x,o,i}$ denote the cartesian components of the corresponding initial values.

6.4.3. Discussion

The time dependences of the position and momentum expectations, Eqs. (6.74), have exactly the form that one expects for a particle exposed to friction, i.e. they describe a particle with an exponentially damped momentum. The mean kinetic energy tends to an asymptotic value, which is also the expected behavior for a dissipative system. However, the asymptotic energy differs from the one given by the equipartition theorem, which is due to the expansion to finite ε-order.

In contrast to that, the equations for the momentum variance, the covariance, and the position variance, Eqs. (6.79), (6.81), and (6.82), look for short times $t \lesssim 1/\eta$ far more complex than a simple phase space diffusion or than the corresponding solution of the QBM master equation, see Eqs. (2.71) and (3.82). Nevertheless, when considering the corresponding equations of motion (6.63), (6.67), and (6.72) with the different constants to first order in ε only, they can be matched with the classical phase space diffusion (2.70). Consequently, the associated solutions (6.79), (6.81), and (6.82) correspond to a phase space diffusion up to order ε.

The full solutions, i.e. including the ε^2-terms, still have some similarities with classical diffusion equations. For one thing, the momentum variance and the covariance tend to fixed values for large times $t \gtrsim 1/\eta$. For another thing, the position variance grows linearly with time in that regime, exactly as one expects from diffusive behavior.

6.5. Decoherence in position

In this section, I turn to the decoherence properties of dissipative collisional decoherence. It will turn out that the position decoherence properties are basically those of the collisional decoherence master equation, while the additional $\hat{\mathbf{P}}$-dependent terms lead to a weak modification only.

At first, consider the master equation in the interaction picture, which was already introduced in Eqs. (3.87). This removes the Hamiltonian part from the master equation (6.50); the remaining terms, which are constituted by the dissipator, then read in position representation,

$$\begin{aligned}\frac{\partial}{\partial t}\langle \boldsymbol{X}|\tilde{\rho}|\boldsymbol{X}'\rangle = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \Bigg\{ \left(\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot(\boldsymbol{X}-\boldsymbol{X}')/\hbar} - 1\right) \frac{3D_p^{\mathrm{K}}}{Q^2} + \frac{D_x^{\mathrm{K}}}{2}\left(\nabla_{\boldsymbol{X}}^2 + \nabla_{\boldsymbol{X}'}^2\right) \\ + \mathcal{A}\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot(\boldsymbol{X}-\boldsymbol{X}')/\hbar}\Bigg[\varepsilon^2\hbar^2\frac{|f_{k_\perp}|^2}{2}\nabla_{\boldsymbol{X}}\cdot\nabla_{\boldsymbol{X}'} + \varepsilon^2\hbar^2\left(\frac{|f|^2}{4p_\beta^4} - \frac{|f_{k_\perp}|^2}{2Q^2}\right)(\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}})(\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}'}) \\ + \mathrm{i}\varepsilon\hbar\frac{|f|^2}{2p_\beta^2}\left(1+\varepsilon\left(1-\frac{Q^2}{4p_\beta^2}\right)\right)\boldsymbol{Q}\cdot(\nabla_{\boldsymbol{X}}-\nabla_{\boldsymbol{X}'}) \\ - \mathrm{i}\varepsilon^2\hbar\frac{k_\perp}{2p_\beta^2}\boldsymbol{Q}\cdot\left(f f_{k_\perp}^*\nabla_{\boldsymbol{X}} - f^* f_{k_\perp}\nabla_{\boldsymbol{X}'}\right)\Bigg]\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot(\boldsymbol{X}-\boldsymbol{X}')/\hbar}\Bigg\}\langle \boldsymbol{X}|\tilde{\rho}|\boldsymbol{X}'\rangle. \quad (6.83)\end{aligned}$$

The first term of the above integrand can be identified with a similar term in the collisional decoherence model, see Eq. (3.87). In fact, in the limit $\varepsilon \to 0$ the above equation exactly coincides with the collisional decoherence version. To estimate the influence of the other terms, I consider a superposition

$$\psi(\boldsymbol{X}) = c_1\psi_1(\boldsymbol{X}) + c_2\psi_2(\boldsymbol{X}) \quad (6.84)$$

of two Gaussian states with $\psi_i(\boldsymbol{X}) = \exp\left(-\left(\boldsymbol{X}-\boldsymbol{X}_i\right)^2/4V_x\right)/\left(2\pi V_x\right)^{3/2}$. The ensuing density matrix consists of four summands,

$$\begin{aligned}\langle \boldsymbol{X}|\tilde{\rho}|\boldsymbol{X}'\rangle = |c_1|^2\,\psi_1(\boldsymbol{X})\psi_1^*(\boldsymbol{X}') + |c_2|^2\,\psi_2(\boldsymbol{X})\psi_2^*(\boldsymbol{X}') \\ + c_1c_2^*\psi_1(\boldsymbol{X})\psi_2^*(\boldsymbol{X}') + c_1^*c_2\psi_1^*(\boldsymbol{X})\psi_2(\boldsymbol{X}'). \quad (6.85)\end{aligned}$$

In the following, I exemplarily analyze the contribution of the first summand of the superposition (6.85) to the decoherence behavior. For this, I use that the momenta Q and $k_\perp$ are of order p_β since they both appear inside the Maxwell–Boltzmann distribution (6.11), which enters via D_x^{K} and $\mathcal{A}$, see Eqs. (6.34) and (6.46). The second term of Eq. (6.83) then becomes

$$\begin{aligned}\frac{D_x^{\mathrm{K}}}{2}\left(\nabla_{\boldsymbol{X}}^2 + \nabla_{\boldsymbol{X}'}^2\right)|c_1|^2\,\psi_1(\boldsymbol{X})\psi_1^*(\boldsymbol{X}') = \frac{\varepsilon^2}{3}\left(|f|^2\,\frac{Q^2}{4p_\beta^2} + |f_{k_\perp}|^2\,p_\beta^2\right) \\ \times\left(\frac{(\boldsymbol{X}-\boldsymbol{X}_1)^2}{2V_x} + \frac{(\boldsymbol{X}'-\boldsymbol{X}_1)^2}{2V_x} - 6\right)\frac{\hbar^2}{4p_\beta^2V_x}\,|c_1|^2\,\psi_1(\boldsymbol{X})\psi_1^*(\boldsymbol{X}'). \quad (6.86)\end{aligned}$$

The factor involving $\hbar$ is rewritten by making use of the relation (3.14) between the variances of a Gaussian state,

$$\frac{\hbar^2}{4p_\beta^2 V_x} = \frac{V_p}{p_\beta^2} \ll 1, \tag{6.87}$$

where the inequality holds for sufficiently high temperatures T because $p_\beta = \sqrt{mk_\mathrm{B}T}$. The terms $\left(\boldsymbol{X}^{(\prime)} - \boldsymbol{X}_1\right)^2 / 2V_x$ in Eq. (6.86) do not grow large as they get suppressed by the Gaussians $\psi_1(\boldsymbol{X}^{(\prime)})$ for large arguments. In sum, the contribution of the term (6.86) to the decoherence behavior is small due to inequality (6.87).

The same analysis can be done for the latter four summands in the integrand of the master equation (6.83). Since every summand contains at least one derivative, one always finds the small term V_p/p_β^2, which turns the whole summand small. This argument also holds for the other three summands in the superposition (6.85), which leads to the insight that the dominant contribution to the positional decoherence is given by the first summand of the integrand in (6.83). But this term produces the same behavior as in the collisional decoherence case, which shows that the dissipative collisional decoherence master equation (6.50) exhibits decoherence in position similar to pure collisional decoherence.

6.6. Widths of the solitons

Through the previous sections we got accustomed to the newly derived master equation (6.50) by investigating its decoherence behavior as well as its friction and diffusion properties. In this last section of this chapter, I turn to the pointer states that are induced by the dissipative collisional decoherence master equation. In a first step, I write down the accompanied NLPSE, which is not easily analytically accessible due to its complexity. One can nevertheless draw some conclusions about the pointer state's shape by applying the Gaussian localization model introduced in the previous chapter. In the same way as for collisional decoherence, one approximates the pointer states as Gaussian states and propagates them with the NLPSE. In the resulting equations of motion for the phase space variances, one then looks for stationary solutions.

Definition of the NLPSE The NLPSE of the master equation in ε-expansion is derived from its general form (3.96),

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{\mathsf{N}}\left[\psi\right]|\psi\rangle = \Bigg[&\frac{1}{\mathrm{i}\hbar}\left(\hat{\mathsf{H}}_0 - \overline{H}_0\right) \\ &+ \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \left(\frac{1}{2}\left(\overline{L^\dagger L} - \hat{\mathsf{L}}^\dagger \hat{\mathsf{L}}\right) + \overline{L^\dagger}\left(\hat{\mathsf{L}} - \overline{L}\right)\right)\Bigg]|\psi\rangle,\end{aligned} \tag{6.88}$$

by using the free Hamiltonian $\hat{\mathsf{H}}_0 = \hat{\mathbf{P}}^2/2M$ and the Lindblad operator (6.35).

Localization model As the first step, I consider a Gaussian state that shall approximate the pointer states,

$$\psi(\boldsymbol{X}) = \frac{1}{(2\pi V_x)^{3/4}} \exp\left(-\frac{1 - \mathrm{i}C_{xp}/\hbar}{4V_x}\boldsymbol{X}^2\right). \tag{6.89}$$

For simplicity, I restrict myself here to spherical Gaussians resting in the phase space origin, $\overline{\boldsymbol{X}} \equiv 0$ and $\overline{\boldsymbol{P}} \equiv 0$. From the spherical symmetry follows that the variance is the same for every cartesian component; for instance, the position variance reads $V_x = \overline{X_i^2}$ for any i.

Secondly, the equation of motion for an hermitian operator $\hat{\mathsf{A}}$, as given by the NLPSE (6.88), is presented. This equation was already given in the general form in the collisional decoherence case in Eq. (5.38); in the present situation, it reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\overline{A} = 2\mathrm{Re}\Bigg\{ &\frac{1}{\mathrm{i}\hbar}\langle\psi|\hat{\mathsf{A}}\hat{\mathsf{H}}_0|\psi\rangle \\ &+ \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \langle\psi|\hat{\mathsf{A}}\left[\frac{1}{2}\left(\overline{L^\dagger L} - \hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}\right) + \overline{L^\dagger}\left(\hat{\mathsf{L}} - \overline{L}\right)\right]|\psi\rangle\Bigg\}. \end{aligned} \tag{6.90}$$

It is useful to evaluate the first summand of dissipative contribution in Eq. (6.90) in advance. The operator product $\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}}$, which appears therein, was already calculated in the course of the derivation of the master equation in Eq. (6.49) and it reads

$$\hat{\mathsf{L}}^\dagger\hat{\mathsf{L}} \cong \frac{3D_p^{\mathrm{K}}}{Q^2} + \frac{D_x^{\mathrm{K}}}{\hbar^2}\hat{\mathbf{P}}^2. \tag{6.91}$$

As usual, the equation is understood below the momenta integrals of $\boldsymbol{Q}$ and $\boldsymbol{k}_\perp$ and the relations derived in Appendix D.1 are applied. In particular, one uses that the terms linear in $\boldsymbol{\lambda}_1$ vanish below the integrals. A short calculation then shows that the integrand of the first summand of the dissipative part in Eq. (6.90) can be put into the simple form,

$$2\mathrm{Re}\left\{\frac{1}{2}\left(\overline{A}\,\overline{L^\dagger L} - \overline{AL^\dagger L}\right)\right\} \cong \frac{D_x^{\mathrm{K}}}{\hbar^2}\mathrm{Re}\left\{3\overline{A}V_p - \overline{A\boldsymbol{P}^2}\right\}. \tag{6.92}$$

Unfortunately, since the position operator dependence does not vanish in the second dissipative contribution, one cannot simplify this term on general grounds. It has to be treated separately for each $\hat{\mathsf{A}}$.

In the next sections, the equations of motion for the position and momentum variances are derived in the context of the localization model.

6.6.1. Position variance

The Hamiltonian part of the equation of motion for $V_x = \overline{X_i^2}$ gives, according to Eq. (6.90),

$$-\frac{1}{2M\hbar}2\mathrm{Re}\left\{\mathrm{i}\overline{X_i^2\boldsymbol{P}^2}\right\} = -\frac{\mathrm{i}}{2M\hbar}\overline{\left[X_i^2, \boldsymbol{P}^2\right]} = \frac{\overline{\{X_i, P_i\}}}{M} = \frac{C_{xp}}{M}. \tag{6.93}$$

First dissipative part The first dissipative contribution is directly infered from Eq. (6.92) and reads

$$2\mathrm{Re}\left\{\frac{1}{2}\left(V_x\overline{L^\dagger L}-\overline{X_i^2 L^\dagger L}\right)\right\}\cong\frac{D_x^{\mathrm{K}}}{\hbar^2}\mathrm{Re}\left\{3V_xV_p-\overline{X_i^2\boldsymbol{P}^2}\right\}. \tag{6.94}$$

One obtains the expectation value $\overline{X_i^2\boldsymbol{P}^2}$ by explicit calculation using the Gaussian state (6.89). Its Laplace operator, which occurs due to the momentum operator, is taken from Eqs. (3.15) and one only needs to solve Gaussian integrals. This is a straightforward task and merely a matter of book-keeping; one gets

$$\begin{aligned}\overline{X_i^2\boldsymbol{P}^2}&=-\hbar^2\int\mathrm{d}\boldsymbol{X}\,|\psi(\boldsymbol{X})|^2\left[-\frac{3}{2V_x}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)X_i^2+\frac{\boldsymbol{X}^2}{4V_x^2}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)^2X_i^2\right]\\&=\frac{3\hbar^2}{2}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)-\frac{5\hbar^2}{4}\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)^2.\end{aligned} \tag{6.95}$$

If one makes use of the variance relation (3.14) of a Gaussian state, the first dissipative contribution (6.94) attains the form

$$2\mathrm{Re}\left\{\frac{1}{2}\left(V_x\overline{L^\dagger L}-\overline{X_i^2L^\dagger L}\right)\right\}\cong\frac{D_x}{\hbar^2}\frac{\hbar^2-C_{xp}^2}{2}. \tag{6.96}$$

Second dissipative part Substituting the Lindblad operator (6.35) into the second dissipative contribution in Eq. (6.90) yields

$$\begin{aligned}2\mathrm{Re}\left\{\overline{L^\dagger}\left(\overline{X_i^2L}-V_x\overline{L}\right)\right\}&=\mathcal{A}2\mathrm{Re}\Bigg\{\left(\lambda_0^*\left\langle\mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle-\boldsymbol{\lambda}_1^*\cdot\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\right\rangle^*\right)\\&\times\left[\lambda_0\left(\left\langle\hat{\mathrm{X}}_i^2\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle-V_x\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle\right)-\boldsymbol{\lambda}_1\cdot\left(\left\langle\hat{\mathrm{X}}_i^2\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\right\rangle-V_x\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\right\rangle\right)\right]\Bigg\},\end{aligned} \tag{6.97}$$

where $\langle\cdot\rangle\equiv\langle\psi|\cdot|\psi\rangle$. The different expectation values that appear in Eq. (6.97) are evaluated by an explicit calculation with the Gaussian state (6.89). Straightforward calculations yield

$$\begin{aligned}\left\langle\mathrm{e}^{\pm\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle&=\mathrm{e}^{-Q^2V_x/2\hbar^2},\\\left\langle\hat{\mathrm{X}}_i^2\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle&=\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle V_x\left(1-\frac{V_xQ_i^2}{\hbar^2}\right),\\\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\right\rangle&=-\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle\frac{1-\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{Q},\\\left\langle\hat{\mathrm{X}}_i^2\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\hat{\mathbf{P}}\right\rangle&=-\left\langle\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle\left[V_x\left(1-\frac{V_xQ_i^2}{\hbar^2}\right)\frac{1-\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{Q}+V_x\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)Q_i\boldsymbol{e}_i\right],\end{aligned} \tag{6.98}$$

where $\boldsymbol{e}_i$ is the cartesian unit vector in i-direction. If one substitutes Eqs. (6.98) into Eq. (6.97), one can write the second dissipative contribution as the following sum of four terms,

$$\begin{aligned}2\mathrm{Re}\left\{\overline{L^\dagger}\left(\overline{X_i^2 L}-V_x\overline{L}\right)\right\} = \mathcal{A}\left|\left\langle \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar}\right\rangle\right|^2 2\mathrm{Re}\Bigg\{ &-|\lambda_0|^2\,\frac{V_x^2Q_i^2}{\hbar^2}\\ &+\lambda_0^*\boldsymbol{\lambda}_1\cdot\left[V_x\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)Q_i\boldsymbol{e}_i-\frac{V_x^2Q_i^2}{\hbar^2}\frac{1-\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{Q}\right]\\ &-\lambda_0\frac{V_x^2Q_i^2}{\hbar^2}\frac{1+\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{\lambda}_1^*\cdot\boldsymbol{Q}\\ &+\boldsymbol{\lambda}_1^*\cdot\boldsymbol{Q}\frac{1+\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{\lambda}_1\cdot\left[V_x\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)Q_i\boldsymbol{e}_i-\frac{V_x^2Q_i^2}{\hbar^2}\frac{1-\mathrm{i}C_{xp}/\hbar}{2}\boldsymbol{Q}\right]\Bigg\}. \end{aligned}\tag{6.99}$$

These summands are now solved one after another by making use of the symmetry properties of the integrand, which are reflected by the relations in Appendix D.1. Notice that $\left|\left\langle\exp\left(\pm\mathrm{i}\boldsymbol{Q}\cdot\hat{\mathbf{X}}/\hbar\right)\right\rangle\right|^2$ does depend on Q^2 only and not on the vector $\boldsymbol{Q}$; therefore, the symmetry properties of the integrand (6.99) are determined solely by the terms inside $\mathrm{Re}\{\cdot\}$. λ_0 does also depend only on the absolute values of the momenta, $k_\perp$ and Q.

From the definition of the kernel D_p^{K} in Eqs. (6.40) together with Eq. (D.15), one infers for the first summand

$$-\,\mathrm{e}^{-Q^2V_x/\hbar^2}D_p^{\mathrm{K}}\frac{2V_x^2}{\hbar^2}. \tag{6.100}$$

To evaluate the second summand, one uses the explicit form of the factor $\boldsymbol{\lambda}_1 = \varepsilon\left(f\boldsymbol{Q}/2p_\beta^2 + f_{k_\perp}\boldsymbol{k}_\perp/k_\perp\right)$ and recalls that all terms linear in $\boldsymbol{k}_\perp$ and odd powers of Q_i vanish below the momenta integrals, see Eqs. (D.10) and (D.12). Additionally, applying Eq. (D.15) allows one to simplify the second summand, which then reads

$$\mathcal{A}\mathrm{e}^{-Q^2V_x/\hbar^2}2\mathrm{Re}\left\{\frac{1}{3}\lambda_0^*\boldsymbol{\lambda}_1\cdot\boldsymbol{Q}\left[V_x\left(1-\frac{\mathrm{i}}{\hbar}C_{xp}\right)-\frac{V_x^2Q^2}{\hbar^2}\frac{1-\mathrm{i}C_{xp}/\hbar}{2}\right]\right\}. \tag{6.101}$$

The same treatment for the third summand of Eq. (6.99) gives the similar result

$$-\,\mathcal{A}\mathrm{e}^{-Q^2V_x/\hbar^2}2\mathrm{Re}\left\{\frac{1}{3}\lambda_0\boldsymbol{\lambda}_1^*\cdot\boldsymbol{Q}\frac{V_x^2Q^2}{\hbar^2}\frac{1+\mathrm{i}C_{xp}/\hbar}{2}\right\}. \tag{6.102}$$

Equations (6.101) and (6.102) taken together, straightforwardly lead to the expression

$$\mathrm{e}^{-Q^2V_x/\hbar^2}\left[\left(2\frac{D_{xp}^{\mathrm{K}}}{\hbar^2}C_{xp}-\eta^{\mathrm{K}}\right)\left(\frac{Q^2V_x}{\hbar^2}-1\right)V_x\right]. \tag{6.103}$$

Finally, the fourth summand gives, after consequent reduction of the $\boldsymbol{k}_\perp$- and $\boldsymbol{Q}$-integrals,

$$-\,\mathcal{A}\mathrm{e}^{-Q^2V_x/\hbar^2}\left[\varepsilon^2\frac{|f|^2\,Q^4}{12p_\beta^2}\left(\frac{Q^2V_x}{2\hbar^2}-1\right)V_x\left(1+\frac{C_{xp}^2}{\hbar^2}\right)\right]. \tag{6.104}$$

One is now in the position to derive the second dissipative contribution by adding up Eqs. (6.100), (6.103), and (6.104). This yields

$$2\mathrm{Re}\left\{\overline{L^\dagger}\left(\overline{X_i L}-\overline{X_i}\,\overline{L}\right)\right\}\cong \mathrm{e}^{-Q^2V_x/\hbar^2}\left[-D_p^{\mathrm{K}}\frac{2V_x^2}{\hbar^2}+\left(2\frac{D_{xp}^{\mathrm{K}}}{\hbar^2}C_{xp}-\eta^{\mathrm{K}}\right)\left(\frac{Q^2V_x}{\hbar^2}-1\right)V_x\right.$$
$$\left.-\varepsilon^2\frac{|f|^2\,Q^4}{12p_\beta^2}\left(\frac{Q^2V_x}{2\hbar^2}-1\right)V_x\left(1+\frac{C_{xp}^2}{\hbar^2}\right)\right]. \quad (6.105)$$

The Hamiltonian and the two dissipative contributions (6.93), (6.96), and (6.105) are put together and give the equation of motion for the position variance,

$$\frac{\mathrm{d}}{\mathrm{d}t}V_x=\frac{C_{xp}}{M}+\int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\left\{\frac{D_x^{\mathrm{K}}}{\hbar^2}\frac{\hbar^2-C_{xp}^2}{2}-\mathrm{e}^{-Q^2V_x/\hbar^2}\left[2\left(D_p^{\mathrm{K}}+\eta^{\mathrm{K}}\frac{Q^2}{2}\right)\frac{V_x^2}{\hbar^2}\right.\right.$$
$$\left.\left.-\eta^{\mathrm{K}}V_x-2\frac{D_{xp}^{\mathrm{K}}}{\hbar^2}C_{xp}\left(\frac{Q^2V_x}{\hbar^2}-1\right)V_x+\mathcal{A}\varepsilon^2\frac{|f|^2\,Q^4}{12p_\beta^4}\left(\frac{Q^2V_x}{2\hbar^2}-1\right)\frac{4V_x^2V_p}{\hbar^2}\right]\right\}. \quad (6.106)$$

6.6.2. Covariance and momentum variance

In the same manner as the position variance, one can derive in a tedious calculation the equation of motion for the covariance, which reads

$$\frac{\mathrm{d}}{\mathrm{d}t}C_{xp}=2\frac{V_p}{M}+\int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\left\{-2\frac{D_x^{\mathrm{K}}}{\hbar^2}V_pC_{xp}-\mathrm{e}^{-Q^2V_x/\hbar^2}\left[2\left(D_p^{\mathrm{K}}+\eta^{\mathrm{K}}\frac{Q^2}{2}\right)\frac{V_xC_{xp}}{\hbar^2}\right.\right.$$
$$\left.\left.-2\frac{D_{xp}^{\mathrm{K}}}{\hbar^2}\left(\frac{Q^2C_{xp}^2}{\hbar^2}-4V_p\right)V_x+\mathcal{A}\varepsilon^2\frac{|f|^2\,Q^4}{12p_\beta^4}\left(\frac{Q^2V_x}{2\hbar^2}-1\right)\frac{4V_xV_p}{\hbar^2}C_{xp}\right]\right\}. \quad (6.107)$$

The equation of motion for the momentum variance V_p is then directly derived from the above two equations by making use of the variance relation (3.14),

$$\frac{\mathrm{d}}{\mathrm{d}t}V_p=\int\mathrm{d}\boldsymbol{Q}\int_{\boldsymbol{Q}_\perp}\mathrm{d}\boldsymbol{k}_\perp\left\{-2\frac{D_x^{\mathrm{K}}}{\hbar^2}V_p^2+\mathrm{e}^{-Q^2V_x/\hbar^2}\left[\left(D_p^{\mathrm{K}}+\eta^{\mathrm{K}}\frac{Q^2}{2}\right)\left(\frac{1}{2}-\frac{C_{xp}^2}{2\hbar^2}\right)\right.\right.$$
$$-\eta^{\mathrm{K}}V_p-2\frac{D_{xp}^{\mathrm{K}}}{\hbar^2}\left(\frac{Q^2}{2}-\left(\frac{Q^2V_x}{\hbar^2}-1\right)V_p\right)C_{xp}$$
$$\left.\left.+2\mathcal{A}\varepsilon^2\frac{|f|^2\,Q^4}{12p_\beta^4}\left(\frac{Q^2V_x}{2\hbar^2}-1\right)\left(\frac{1}{2}-\frac{C_{xp}^2}{2\hbar^2}\right)V_p\right]\right\}. \quad (6.108)$$

6.6.3. Stationary solutions

Equations (6.106)-(6.108) provide a set of coupled nonlinear integro-differential equations, which one cannot hope to solve, in general. However, a great simplification is

achieved by considering terms up to order ε only. As a reminder, the dependence on ε can be read off the definition of the kernels D_p^{K}, D_x^{K}, η^{K}, and D_{xp}^{K}, which is given in Eqs. (6.40), (6.46), (6.42), and (6.43) respectively. There, one remarks that only D_p^{K} and η^{K} contribute in this approximation.

Before simplifying the equations of motion for the variances, I introduce dimensionless units, which will prove convenient for the following discussion. These units are defined very similarly to the ones used in the collisional decoherence chapter and read

$$\mathrm{T} = \frac{1}{\eta}, \quad \mathrm{L} = \frac{\hbar}{p_\beta}, \quad \mathrm{P} = p_\beta. \tag{6.109}$$

Here, η is the friction constant, see Eq. (6.42), and p_β is the most probable momentum of the environmental gas particles, see Eq. (6.4). These units give rise to a dimensionless parameter, which I denote by the same symbol as the collisional decoherence parameter,

$$\zeta = \frac{p_\beta^2}{\hbar M \eta}. \tag{6.110}$$

With the dimensionless scales (6.109) and by keeping terms up to first order in ε only, the set (6.106)-(6.108) is straightforwardly rewritten into the much simpler form

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} V_x &= \zeta C_{xp} - 2\tilde{D}_{V_x} V_x^2 + \tilde{\eta}_{V_x} V_x, \\ \frac{\mathrm{d}}{\mathrm{d}t} V_p &= \tilde{D}_{V_x} \frac{1 - C_{xp}^2}{2} - \tilde{\eta}_{V_x} V_p, \\ \frac{\mathrm{d}}{\mathrm{d}t} C_{xp} &= 2\zeta V_p - 2\tilde{D}_{V_x} V_x C_{xp}, \end{aligned} \tag{6.111}$$

where I introduced the V_x-dependent values

$$\begin{aligned} \tilde{\eta}_{V_x} &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mathrm{e}^{-Q^2 V_x} \eta^{\mathrm{K}}, \\ \tilde{D}_{V_x} &= \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mathrm{e}^{-Q^2 V_x} \left(D_p^{\mathrm{K}} + \eta^{\mathrm{K}} \frac{Q^2}{2} \right). \end{aligned} \tag{6.112}$$

The set (6.111) resembles the corresponding set derived for collisional decoherence, see Eqs. (5.50) and (5.56), the differences being that the latter does not contain $\tilde{\eta}_{V_x}$ and that $\tilde{D}_{V_x}$ has a particular form defined by the Gaussian momentum kick distribution.

The equations for the variances further simplify if one keeps in $\tilde{D}_{V_x}$ the leading order term in ε only. From the definitions (6.40) and (6.42) of D_p^{K} and η^{K}, one infers that $\tilde{\eta}_{V_x}$ and $\tilde{D}_{V_X}$ get proportional in this case:

$$\tilde{D}_{V_x} = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \mathrm{e}^{-Q^2 V_x} \frac{\mathcal{A}}{3} |f|^2 Q^2 = \frac{\tilde{\eta}_{V_x}}{\varepsilon}. \tag{6.113}$$

To calculate the stationary variances of the soliton, one needs to set the left-hand sides of Eqs. (6.111) to zero and after some algebra, one can arrive at

$$\zeta = \tilde{D}_{V_x} V_x \sqrt{4V_x^2 - \varepsilon^2}. \tag{6.114}$$

Conclusion can only be drawn from this equation, if one further characterizes the V_x-dependent integral $\tilde{D}_{V_X}$. Motivated by the corresponding form in the collisional decoherence case, I rewrite the integral (6.113) and arrive at

$$\tilde{D}_{V_x} = \frac{2}{3}\int \mathrm{d}\boldsymbol{Q} \mathrm{e}^{-Q^2 V_x} Q^2 G(Q), \tag{6.115}$$

with the kick distribution,

$$G(Q) = \frac{g}{\pi^{3/2} Q}\int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \left|f\left(k_\perp, Q\right)\right|^2 \mathrm{e}^{-\left(k_\perp^2 + Q^2/4\right)}, \tag{6.116}$$

where $g = n_{\mathrm{gas}}\hbar^2/m\eta p_\beta$.

Gaussian kick distribution In the collisional decoherence case discussed in the previous chapter, $G(Q)$ is assumed to be a normalized centered Gaussian,

$$G(Q) = \frac{\mathrm{e}^{-Q^2/2}}{(2\pi)^{3/2}}, \tag{6.117}$$

with the consequence that in three dimensions solitons exist only for particular parameter values. Upon using this Gaussian distribution to calculate the integral (6.115), the width equation (6.114) attains the form

$$\zeta = \frac{2V_x\sqrt{4V_x^2 - \varepsilon^2}}{(1+2V_x)^{5/2}}, \tag{6.118}$$

which is very similar to the form of the corresponding equation for 3D collisional decoherence, see Eq. (5.59). In fact, both equations coincide up to a constant factor in the non-dissipative limit, $\varepsilon = 0$. Equation (6.118) is plotted in Fig. 6.2 for $\varepsilon = 0.001$; one infers that solitons exist up to a critical parameter $\zeta_{1,\mathrm{crit}} \approx 0.286$ only, with the finite variance $V_x(\zeta_{1,\mathrm{crit}}) \approx 2$. The inclusion of dissipative terms, via a nonvanishing ε, leads to a lower bound for the variance V_x. However, dissipation does not lead to qualitatively different behavior for large ζ.

Non-Gaussian kick distribution By using a kick distribution that is non-Gaussian, one may arrive at an equation for the soliton width, which has solutions for all ζ. In particular, I make the ansatz

$$G(Q) = \frac{\mathrm{e}^{-Q^2/2}}{(2\pi)^{3/2} Q^2}, \tag{6.119}$$

for the momentum kick distribution. Like in the previous paragraph, using Eqs. (6.114) and (6.115) one arrives at the width equation

$$\zeta = \frac{2V_x\sqrt{4V_x^2 - \varepsilon^2}}{(1+2V_x)^{3/2}}, \tag{6.120}$$

which is also plotted in Fig. 6.2. One observes that for small ζ there exists the same lower bound for V_x and for large ζ the soliton always attains a finite size.

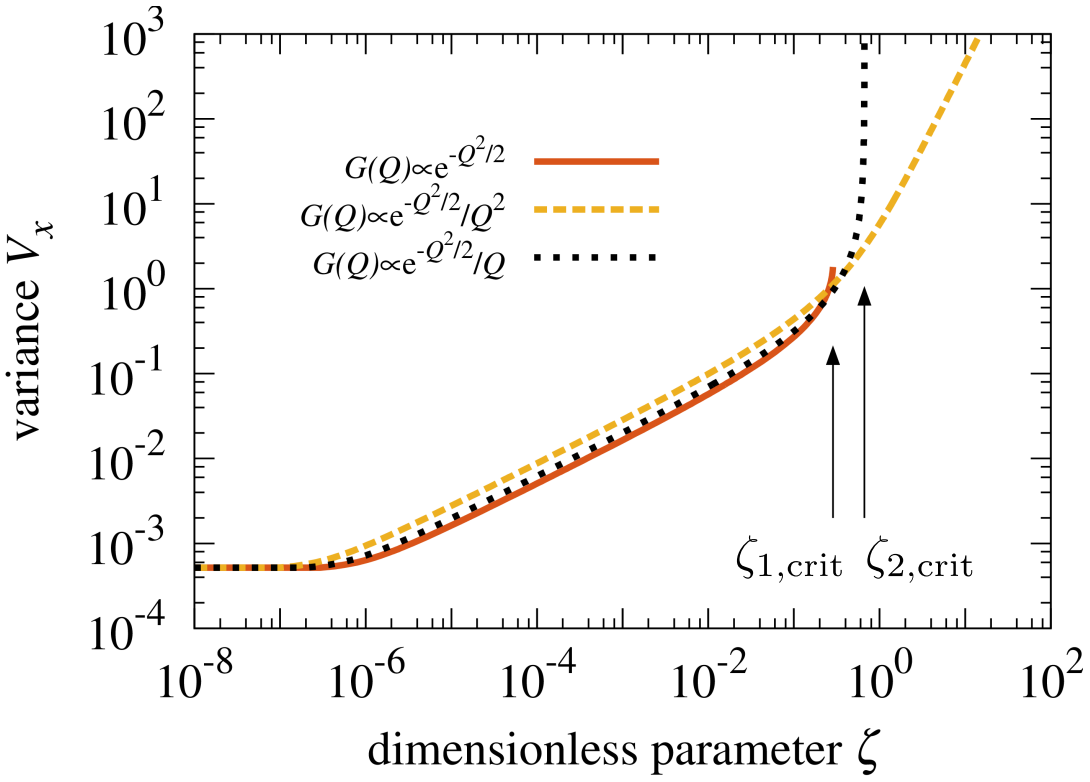

Figure 6.2.: Solitonic width depending on the dimensionless parameter ζ for different momentum kick distributions $G(Q)$: a Gaussian distribution (solid, red), a Gaussian divided by Q^2 (dashed, yellow), and a Gaussian divided by Q (dashed, black). The mass parameter is $\varepsilon = 0.001$.

Hard-sphere scattering As a final example, one may calculate the momentum kick distribution by means of a particular scattering cross section via Eq. (6.116). For scattering off a hard-sphere of diameter d, one can approximate the differential scattering cross-section for small scattering angles and large energies [78]:[2]

$$|f(k_\perp, Q)|^2 \approx \frac{d^4}{4}\left(k_\perp^2 + \frac{Q^2}{4}\right)\exp\left(-\frac{Q^2 d^2}{4}\right). \tag{6.121}$$

Inserting $|f(k_\perp, Q)|^2$ into the integral (6.116), one can directly evaluate the $\boldsymbol{k}_\perp$-integral and arrives at a modified Gaussian function for the momentum kick distribution,

$$G(Q) = \frac{g d^4}{16\pi}\left(\frac{1}{Q} + \frac{Q}{2}\right)\mathrm{e}^{-Q^2\left(1+d^2\right)/4}. \tag{6.122}$$

The dominating term in Eq. (6.122) is the $1/Q$-term and the constant prefactor has no influence on the qualitative behavior of the width equation (6.114). For the sake of simplicity, I therefore make the ansatz

$$G(Q) = \frac{\mathrm{e}^{-Q^2/2}}{4\pi Q}, \tag{6.123}$$

for the kick distribution. Together with Eqs. (6.114) and (6.115) this yields

$$\zeta = \frac{4V_x\sqrt{4V_x^2 - \varepsilon^2}}{3\left(1 + 2V_x\right)^2}. \tag{6.124}$$

The corresponding graph is shown in Fig. 6.2. One observes that above the critical parameter $\zeta_{2,\mathrm{crit}} = 2/3$ there exist no solitons; the variance diverges at this point, $V_x(\zeta_{2,\mathrm{crit}}) \to \infty$.

6.7. Summary

In this last chapter, I presented the QLBE as a Lindblad master equation describing a test particle's interaction with an ideal gaseous environment via the corresponding elastic scattering amplitudes. I showed that the QLBE generalizes the master equation of QBM and that of collisional decoherence in the sense that it incorporates both cases as limits. For instance, the non-dissipative collisional decoherence limit is attained in the limit of an infinite test particle mass, i.e. $\varepsilon = m/M \to 0$.

A further step towards the characterization of the full QLBE is then taken by considering a very massive test particle with finite mass, $\varepsilon > 0$. On this basis, I derived a Lindblad master equation by a Taylor expansion of the Lindblad operators of the QLBE

[2] In [78], the scattering cross-section is given as a function of the scattering angle ϑ and the momentum p. For switching to the variables $k_\perp$ and Q, I use Fig. 6.1 to derive the two identities $p^2 = k_\perp^2 + Q^2/4$ and $2\left(1 - \cos\vartheta\right)p^2 = Q^2$ and apply the small angle approximation $1 - \cos\vartheta \approx \vartheta^2/2$.

to first order in ε. This dissipative collisional decoherence master equation leads to decoherence in position in a similar manner as the pure collisional decoherence master equation. Moreover, I showed with the help of the exponentially damped momentum expectation value that this master equation also exhibits friction. The position variance grows linearly with time for large times, exactly as one would expect from a diffusive equation. One can therefore say that the dissipative collisional decoherence generalizes collisional decoherence and QBM, since it incorporates main features of both models.

In the last section, I applied the localization model based on propagating Gaussian states via the NLPSE and derived approximate equations of motion to estimate the pointer state's stationary position variance. It turns out that the main effect of the incorporation of friction lies in a lower bound of the position variance for small dimensionless parameters ζ. However, the behavior of the solitons that they exist up to a critical parameter only, is not changed in comparison with the collisional decoherence case. Nevertheless, one can find situations, where there exist pointer states for all parameters ζ, by changing the momentum kick distribution from a Gaussian (as used in collisional decoherence) to a Gaussian divided by Q^2.

7. Conclusions

In the course of this thesis, the quantum-to-classical transition of a dissipative open quantum system was elucidated by using the pointer state unraveling, which is a particular piecewise deterministic stochastic process in Hilbert space representing the evolution of a Lindblad master equation. Specifically, I identified the pointer states of quantum Brownian motion to be rotated Gaussians in phase space. Superpositions of pointer states turn into a mixture with probabilities given by Born's rule. Furthermore, the pointer states move on stochastic trajectories that may be described by a diffusion process in phase space with an exponentially damped momentum. Crucially, in the semiclassical limit, the pointer states become more localized and may be identified with points in phase space. Their phase space trajectory then turns into the Langevin equation of classical Brownian motion. On these grounds, we have attained a clear and convenient picture of how classical behavior emerges from a purely quantum mechanical point of view. Moreover, it became clear how classical stochasticity may be produced by the interplay between the deterministic and the stochastic part of the unraveling's quantum trajectories. All that led to a better understanding under what circumstances the quantum motion of a test particle can be approximately described by classical means.

The above results serve as a demonstration for the worthiness of the pointer state unraveling, which was already indicated by the successful application to the one-dimensional collisional decoherence master equation [37–39]. Since solutions of the master equation in two and three dimensions are not obtained by a simple product ansatz of one-dimensional solutions, an analysis of the pointer states of multi-dimensional collisional decoherence was presented. I gained analytic expressions for the pointer state width in all considered dimensions by approximating them with Gaussian states. Unexpectedly, in two and three dimensions, pointer states do not exist for all values of the dimensionless coupling strength parameter, which is in sharp contrast to the one-dimensional treatment, cf. [37–39]. It turns out that the existence of pointer states depends on the form of the momentum kick distribution of the environmental gas particles. For instance, in the collisional decoherence model a Gaussian distribution is used. However, using a modified Gaussian kick distribution can resolve this problem and lead to pointer states for all parameter values.

Collisional decoherence describes the short-time behavior of a massive test particle and therefore does not include friction effects. To arrive at a master equation that incorporates friction, one has to treat the environmental coupling on more general grounds. This can be done on a systematic level by an expansion of the quantum linear Boltzmann equation in the mass ratio between the gas particles and the test particle. The quantum linear Boltzmann equation describes the motional state of a marker particle immersed in an ideal gaseous environment solely on basis of the scattering amplitudes [25]. For a

vanishing mass ratio, one arrives at the non-dissipative collisional decoherence master equation. An expansion of the Lindblad operators of the quantum linear Boltzmann equation to first order in the aforementioned mass ratio yielded a dissipative master equation. I denoted it as the master equation of *dissipative collisional decoherence* because it may be seen as the "natural" dissipative extension of collisional decoherence. It predicts decoherence in position similar to the collisional decoherence master equation. On the other hand, its momentum expectation value is exponentially damped and the position variance grows asymptotically linear with time. Thus the master equation describes frictional and diffusive behavior.

Equations of motion for the variances of the pointer states of dissipative collisional decoherence were obtained by applying the approximation and propagation via Gaussian states that I introduced and tested in the context of collisional decoherence. The extracted width shows qualitatively the same behavior regarding the existence of pointer states as its non-dissipative counterpart. Nonetheless, in difference to pure collisional decoherence, the dissipative extensions give rise to a lower bound for the pointer state width.

Beyond the scope of this thesis, it is interesting to investigate whether the similarity between dissipative collisional decoherence and pure collisional decoherence also holds when it comes to the behavior of the pointer state tails. Specifically, since the pointer states of pure collisional decoherence are exponentially localized, one may expect the same in the dissipative extension. A numerical investigation of these aspects would require an implementation of the nonlinear pointer state equation of dissipative collisional decoherence, which is far more complex than that of pure collisional decoherence, for instance, due to the necessity to incorporate and evaluate the scattering amplitudes for a specific interaction potential. Besides a proper characterization of the pointer states, it is also of interest to look at the full unraveling of dissipative collisional decoherence and investigate the equations of motion its pointer states follow. Here, the natural question arises whether the diffusive behavior, which was seen on the master equation level, also shows up for the pointer state trajectories. One is tempted to assume that diffusive behavior is produced by a similar mechanism as in the quantum Brownian motion case, which should be clarified by a thorough analysis of the accompanied pointer state unraveling. Finally, the unraveling should give a classical equation of motion in the semiclassical limit; in this particular case, I expect it to be a classical jump equation derived from the classical linear Boltzmann equation, in the same mass expansion that led to the quantum master equation. All this would give a better, i.e. more refined, understanding of the quantum-to-classical correspondence of particle motion.

Appendix

A. Classical stochastic processes

A.1. Statistics of estimators of phase space diffusion

The statistical properties of the estimators (4.40) of the phase space diffusion shall be derived. To repeat, the SDE of phase space diffusion is given by Eq. (2.63) in Section 2.4 and reads

$$\begin{pmatrix} \mathrm{d}x \\ \mathrm{d}p \end{pmatrix} = \begin{pmatrix} p \\ -p \end{pmatrix} \mathrm{d}t + \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} \mathrm{d}W_1 \\ \mathrm{d}W_2 \end{pmatrix}. \tag{A.1}$$

The corresponding ensemble mean values $\mathrm{E}[x]$, $\mathrm{E}[p]$ and the ensemble variances $\mathrm{Var}[x]$, $\mathrm{Var}[p]$, and $\mathrm{Cov}[x,p]$ are given in Eqs. (2.66) and (2.71). For a sample of N trajectories of this stochastic process, one may use the unbiased estimators given by Eqs. (4.40):

$$\begin{aligned} m_N[x] &= \frac{1}{N}\sum_{i=1}^{N} x_i, \\ m_N[p] &= \frac{1}{N}\sum_{i=1}^{N} p_i, \\ s_N^2[x] &= \frac{1}{N-1}\sum_{i=1}^{N} \left(x_i - m_N[x]\right)^2, \\ s_N^2[p] &= \frac{1}{N-1}\sum_{i=1}^{N} \left(p_i - m_N[p]\right)^2, \\ c_N[x,p] &= \frac{1}{N-1}\sum_{i=1}^{N} \left(x_i - m_N[x]\right)\left(p_i - m_N[p]\right), \end{aligned} \tag{A.2}$$

where x_i and p_i are the position and momentum of trajectory i. The estimators (A.2) are themselves stochastic values and it is the purpose of this section to derive their (ensemble) mean values as well as their variances.

A.1.1. Mean values

The mean value of the position estimator equals its ensemble mean value,

$$\mathrm{E}\left[m_N[x]\right] = \frac{1}{N}\sum_{i=1}^{N} \mathrm{E}\left[x_i\right] = \mathrm{E}\left[x\right]. \tag{A.3}$$

Similarly, one gets for the momentum estimator, $\mathrm{E}\left[m_N[p]\right] = \mathrm{E}\left[p\right]$. The corresponding calculations for the ensemble averages of the variance estimators are a little bit more involved but yield similar results. For instance, for the ensemble mean of the position variance estimator one evaluates,

$$\begin{aligned}\mathrm{E}\left[s_N^2[x]\right] &= \frac{1}{N-1}\sum_{i=1}^{N}\mathrm{E}\left[\left(x_i - m_N[x]\right)^2\right] \\ &= \frac{1}{N-1}\sum_{i=1}^{N}\left(\mathrm{E}[x_i^2] - \frac{2}{N}\sum_{j=1}^{N}\mathrm{E}\left[x_i x_j\right] + \frac{1}{N^2}\sum_{j,k=1}^{N}\mathrm{E}\left[x_j x_k\right]\right) \\ &= \mathrm{Var}\left[x\right]. \end{aligned} \tag{A.4}$$

In the third line, I used that the x_i are independent stochastic processes and therefore I may factorize the ensemble averages involving products of them:

$$\begin{aligned}\mathrm{E}\left[x_j x_k\right] &= \mathrm{E}\left[x_j\right]\mathrm{E}\left[x_k\right] + \delta_{jk}\left(\mathrm{E}\left[x_j^2\right] - \mathrm{E}\left[x_j\right]^2\right) \\ &= \mathrm{E}\left[x\right]^2 + \delta_{jk}\mathrm{Var}\left[x\right]. \end{aligned} \tag{A.5}$$

Analogously, one derives

$$\begin{aligned}\mathrm{E}\left[s_N^2[p]\right] &= \mathrm{Var}\left[p\right], \\ \mathrm{E}\left[c_N[x,p]\right] &= \mathrm{Cov}\left[x,p\right]. \end{aligned} \tag{A.6}$$

The derivation of the ensemble variance of the estimators (A.2) is, in general, a more lengthy task as can be seen in the following section.

A.1.2. Variances of the mean estimators

Direct calculation One possible way of calculating the variance of the mean value estimators is by direct evaluation,

$$\mathrm{Var}[m_N[x]] = \mathrm{Var}[\frac{1}{N}\sum_{i=1}^{N}x_i] = \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Var}[x_i] = \frac{\mathrm{Var}[x]}{N}. \tag{A.7}$$

To see this, I first used that constants can be put outside the variance operation by taking their square. Secondly, I made use of the fact that the variance of a sum of *independent* stochastic variables equals the sum of the individual variances, which is confirmed by the simple calculation for the two independent processes a and b,

$$\begin{aligned}\mathrm{Var}\left[a+b\right] &= \mathrm{E}\left[a^2 + b^2 + 2ab\right] - \left(\mathrm{E}\left[a\right] + \mathrm{E}\left[b\right]\right)^2 \\ &= \mathrm{E}\left[a^2\right] + \mathrm{E}\left[b^2\right] + 2\mathrm{E}\left[a\right]\mathrm{E}\left[b\right] - \mathrm{E}\left[a\right]^2 - \mathrm{E}\left[b\right]^2 - 2\mathrm{E}\left[a\right]\mathrm{E}\left[b\right] \\ &= \mathrm{Var}\left[a\right] + \mathrm{Var}\left[b\right]. \end{aligned} \tag{A.8}$$

Of course, the calculation for the momentum estimator yields the same result. Unfortunately, if the estimator cannot be written as a sum of independent stochastic processes,

the above reasoning is not applicable. Although the independence condition is valid for the variance of $m_N[p]$ as well as for the covariance between $m_N[x]$ and $m_N[p]$, in the following, I calculate their variance via the derivation of the appropriate SDE. This serves as an illustration for the derivation of the ensemble variances of the variance estimators, where the above independence condition does not hold.

Calculation via SDEs The variance of the momentum estimator is $\mathrm{Var}[m_N[p]] = \mathrm{E}[m_N[p]^2] - \mathrm{E}[p]^2$, hence its equation of motion reads

$$\mathrm{dVar}[m_N[p]] = \mathrm{E}[\mathrm{d}\left(m_N[p]^2\right)] - 2\mathrm{E}[p]\mathrm{E}[\mathrm{d}p]. \tag{A.9}$$

The SDE for $m_N[p]^2$ that appears in the above formula, is derived from the SDE for $m_N[p]$,

$$\mathrm{d}m_N[p] = -m_N[p]\mathrm{d}t + \frac{1}{N}\sum_{i=1}^{N}\left(B_{21}\mathrm{d}W_{1,i} + B_{22}\mathrm{d}W_{2,i}\right), \tag{A.10}$$

where the sum goes over the N different trajectories and $\mathrm{d}W_{1,i}$ and $\mathrm{d}W_{2,i}$ are independent Wiener increments. Equation (A.10) is readily obtained from the stochastic model (A.1) together with the definition of the estimators (A.2). The SDE for the corresponding second moment is derived by using $\mathrm{d}\left(m_N[p]^2\right) = 2m_N[p]\mathrm{d}m_N[p] + \left(\mathrm{d}m_N[p]\right)^2$,

$$\mathrm{d}\left(m_N[p]^2\right) = \left(-2m_N[p]^2 + \frac{B_{21}^2 + B_{22}^2}{N}\right)\mathrm{d}t + \frac{2}{N}m_N[p]\sum_{i=1}^{N}\left(B_{21}\mathrm{d}W_{1,i} + B_{22}\mathrm{d}W_{2,i}\right). \tag{A.11}$$

Finally, from Eqs. (A.9) and (A.11) together with $\mathrm{E}[\mathrm{d}p] = -\mathrm{E}[p]\mathrm{d}t$ from Eqs. (2.65), one obtains the equation of motion of the variance of the momentum estimator

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[m_N[p]] = -2\mathrm{Var}[m_N[p]] + \frac{D_p}{N}, \tag{A.12}$$

where the diffusion constant $D_p = B_{21}^2 + B_{22}^2$ is used, see Eqs. (2.69). Notice that the second term of Eq. (A.11) vanishes in the ensemble mean since $m_N[p]$ is non-anticipating and thus stochastically independent of the Wiener increments.

Following the same steps, one can derive the two differential equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[m_N[x]] &= 2\mathrm{Cov}[m_N[x], m_N[p]] + \frac{D_x}{N},\\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cov}[m_N[x], m_N[p]] &= -\mathrm{Cov}[m_N[x], m_N[p]] + \mathrm{Var}[m_N[p]] + \frac{D_{xp}}{N}.\end{aligned} \tag{A.13}$$

A comparison of Eqs. (A.12) and (A.13) with the differential equations for the ensemble variances, Eqs. (2.70), shows that they are identical except for the diffusion constants,

which are scaled by the sample size N. Consequently, the solutions of the former are proportional to those of the latter and can be read off Eqs. (2.71). One gets

$$\begin{aligned} \mathrm{Var}[m_N[x]] &= \frac{\mathrm{Var}[x]}{N}, \\ \mathrm{Var}[m_N[p]] &= \frac{\mathrm{Var}[p]}{N}, \\ \mathrm{Cov}[m_N[x], m_N[p]] &= \frac{\mathrm{Cov}[x,p]}{N}. \end{aligned} \tag{A.14}$$

A.1.3. Variances of the variance estimators

The ensemble variance of the momentum variance estimator is derived along the same lines as in the previous section. Exemplarily, I derive the ensemble variance of $s_N^2[p]$. At first, one rewrites this estimator into the more convenient form,

$$s_N^2[p] = \frac{1}{N-1}\sum_{i=1}^{N} p_i^2 - \frac{N}{N-1} m_N[p]^2. \tag{A.15}$$

From this form, one can easily see that $s_N^2[p]$ is not writable as a sum of independent stochastic values since $m_N[p]$ is stochastically dependent on each p_i. Therefore the simple argument from the previous section does not hold.

In a second step, by using Eqs. (A.1) and (A.11), one derives the SDE

$$\begin{aligned} \mathrm{d}s_N^2[p] &= \frac{1}{N-1}\sum_{i=1}^{N}\left(2p_i\mathrm{d}p_i + (\mathrm{d}p_i)^2\right) - \frac{N}{N-1}\mathrm{d}\left(m_N[p]^2\right) \\ &= \left(D_p - 2s_N^2[p]\right)\mathrm{d}t + \frac{2}{N-1}\mathrm{d}Z, \end{aligned} \tag{A.16}$$

with the stochastic process

$$\begin{aligned} \mathrm{d}Z &= \sum_i^N \left(p_i - m_N[p]\right)\left(B_{21}\mathrm{d}W_{1,i} + B_{22}\mathrm{d}W_{2,i}\right) \\ &= \sqrt{(N-1)\,\mathrm{Var}[p]D_p}\,\mathrm{d}\tilde{W}. \end{aligned} \tag{A.17}$$

The process $\mathrm{d}Z$ is proportional to the Wiener process $\mathrm{d}\tilde{W}$, which can be shown by using that the factor $p_i - m_N[p]$ is non-anticipating. It is therefore easy to evaluate all moments of $\mathrm{d}Z$ and confirm the statement.

In another step, one infers the SDE for $s_N^2[p]^2$ from Eqs. (A.16) and (A.17)

$$\begin{aligned} \mathrm{d}\left(s_N^2[p]^2\right) = \left(2D_p s_N^2[p] - 4s_N^2[p]^2 + \frac{4D_p\mathrm{Var}[p]}{N-1}\right)\mathrm{d}t \\ + 4\sqrt{\frac{D_p\mathrm{Var}[p]}{N-1}}s_N^2[p]\mathrm{d}\tilde{W}. \end{aligned} \tag{A.18}$$

The differential equation for the variance of the variance estimator is now directly accessible via the relation

$$\mathrm{dVar}[s_N^2[p]] = \mathrm{E}[\mathrm{d}\left(s_N^2[p]^2\right)] - 2\mathrm{Var}[p]\mathrm{dVar}[p]. \tag{A.19}$$

Together with Eqs. (2.70) and (A.16), this finally gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[s_N^2[p]] = -4\mathrm{Var}[s_N^2[p]] + \frac{4D_p\mathrm{Var}[p]}{N-1}. \tag{A.20}$$

Other estimators Following the above calculations, one can obtain the differential equations for the ensemble variances of $s_N^2[x]$ and $c_N[x,p]$. Unfortunately, the situation is more complex than in the above case, such that the desired differential equations involve different covariances of the estimators. Before writing down the differential equations that one needs to solve, I introduce the abbreviations

$$\begin{aligned} Y_1 &= \mathrm{Cov}[s_N^2[p], c_N[x,p]], \\ Y_2 &= \mathrm{Cov}[s_N^2[x], c_N[x,p]], \\ Y_3 &= \mathrm{Cov}[s_N^2[x], s_N^2[p]]. \end{aligned} \tag{A.21}$$

For the equations of motion of the variances of the two estimators, one then gets by staightforward calculations,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[c_N[x,p]] &= -2\mathrm{Var}[c_N[x,p]] + 2Y_1 \\ &\quad + \frac{D_x\mathrm{Var}[p] + D_p\mathrm{Var}[x] + 2D_{xp}\mathrm{Cov}[x,p]}{N-1}, \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}[s_N^2[x]] &= 4Y_2 + \frac{4D_x\mathrm{Var}[x]}{N-1}. \end{aligned} \tag{A.22}$$

The three equations of motion for the covariances (A.21) are obtained in the same way,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}Y_1 &= -3Y_1 + \mathrm{Var}[s_N^2[p]] + \frac{2\left(D_p\mathrm{Cov}[x,p] + D_{xp}\mathrm{Var}[p]\right)}{N-1}, \\ \frac{\mathrm{d}}{\mathrm{d}t}Y_2 &= -Y_2 + Y_3 + 2\mathrm{Var}[c_N[x,p]] + \frac{2\left(D_x\mathrm{Cov}[x,p] + D_{xp}\mathrm{Var}[x]\right)}{N-1}, \\ \frac{\mathrm{d}}{\mathrm{d}t}Y_3 &= -2Y_3 + 2Y_1 + \frac{4D_{xp}\mathrm{Cov}[x,p]}{N-1}. \end{aligned} \tag{A.23}$$

Equations (A.20), (A.22), and (A.23) form a closed set of six differential equations that can be solved consecutively by direct integration. A long and tedious calculation gives

the solutions, which I present in the order they are obtained:

$$\begin{aligned}
&&\mathrm{Var}[s_N^2[p]] &= \frac{2}{N-1}\mathrm{Var}[p]^2, \\
Y_1 = &\quad \mathrm{Cov}[s_N^2[p], c_N[x,p]] &&= \frac{2}{N-1}\mathrm{Var}[p]\mathrm{Cov}[x,p], \\
&&\mathrm{Var}[c_N[x,p]] &= \frac{1}{N-1}\left(\mathrm{Var}[x]\mathrm{Var}[p] + \mathrm{Cov}[x,p]^2\right), \\
Y_3 = &\quad \mathrm{Cov}[s_N^2[x], s_N^2[p]] &&= \frac{2}{N-1}\mathrm{Cov}[x,p]^2, \\
Y_2 = &\quad \mathrm{Cov}[s_N^2[x], c_N[x,p]] &&= \frac{2}{N-1}\mathrm{Var}[x]\mathrm{Cov}[x,p], \\
&&\mathrm{Var}[s_N^2[x]] &= \frac{2}{N-1}\mathrm{Var}[x]^2.
\end{aligned} \tag{A.24}$$

It is easy to validate these formulas by differentiation and insertion of Eqs. (2.70).

B. Dynamics of open quantum systems

B.1. Derivation of the Lindblad form

The derivation presented in this section is motivated by Ref. [42].

In order to construct the general form of the Lindblad generator $\mathcal{L}$, see Eqs. (3.29) and (3.30), I consider a finite dimensional system Hilbert space, i.e. $\dim \mathcal{H}_\mathrm{S} = N$. Moreover, one chooses an orthonormal operator basis $\hat{\mathsf{F}}_i$, with $i = 1, 2, \ldots, N^2$, which fulfills the orthonormality condition

$$\left(\hat{\mathsf{F}}_i, \hat{\mathsf{F}}_j\right) \equiv \mathrm{Tr}\left[\hat{\mathsf{F}}_i^\dagger \hat{\mathsf{F}}_j\right] = \delta_{ij}, \tag{B.1}$$

where the trace is over $\mathcal{H}_\mathrm{S}$. Starting from a dynamical semigroup mapping for system density matrices ρ in Kraus representation, see Eqs. (3.22),

$$\mathcal{M}_t\left[\rho\right] = \sum_{\alpha,\beta} \hat{\mathsf{W}}_{\alpha,\beta}(t) \rho \hat{\mathsf{W}}_{\alpha,\beta}^\dagger(t), \tag{B.2}$$

one can rewrite this with the help of the orthonormal operator basis $\hat{\mathsf{F}}_i$. To this end, it is convenient to set $\hat{\mathsf{F}}_{N^2} = \mathbb{1}_\mathrm{S}/\sqrt{N}$, so that all other $\hat{\mathsf{F}}_i$ are traceless. The Kraus operators (3.23) then read

$$\hat{\mathsf{W}}_{\alpha,\beta}(t) = \sum_i \hat{\mathsf{F}}_i \left(\hat{\mathsf{F}}_i, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right), \tag{B.3}$$

and Eq. (B.2) takes the form

$$\mathcal{M}_t\left[\rho\right] = \sum_{i,j} c_{ij} \hat{\mathsf{F}}_i \rho \hat{\mathsf{F}}_j^\dagger, \tag{B.4}$$

with coefficients

$$c_{ij} = \sum_{\alpha,\beta} \left(\hat{\mathsf{F}}_i, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right) \left(\hat{\mathsf{F}}_j, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right)^*. \tag{B.5}$$

From the definition of the c_{ij} it is clear that $c_{ij} = c_{ji}^*$.

In a next step, one uses the representation of the semigroup mapping via its generator $\mathcal{L}$, see Eq. (3.28), which yields

$$\begin{aligned}\mathcal{L}[\rho] &= \lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \left(\mathcal{M}_\varepsilon - \mathbb{1}_\mathrm{S}\right)[\rho] \\ &= \lim_{\varepsilon\to 0} \left(\frac{c_{N^2N^2} - N}{\varepsilon N} \rho + \frac{1}{\varepsilon\sqrt{N}} \sum_{i=1}^{N^2-1} \left(c_{iN^2} \hat{\mathsf{F}}_i \rho + c_{iN^2}^* \rho \hat{\mathsf{F}}_i^\dagger \right) + \sum_{i,j=}^{N^2-1} \frac{c_{ij}}{\varepsilon} \hat{\mathsf{F}}_i \rho \hat{\mathsf{F}}_j^\dagger \right).\end{aligned} \tag{B.6}$$

The generator is further rewritten by defining the quantities

$$\begin{aligned} a_{N^2N^2} &= \lim_{\varepsilon\to 0}\frac{c_{N^2N^2}-N}{\varepsilon}, \\ a_{iN^2} &= \lim_{\varepsilon\to 0}\frac{c_{iN^2}}{\varepsilon}, \quad i=1,\dots,N^2-1, \\ a_{ij} &= \lim_{\varepsilon\to 0}\frac{c_{ij}}{\varepsilon}, \quad i,j=1,\dots,N^2-1, \\ \hat{\mathsf{F}} &= \frac{1}{\sqrt{N}}\sum_{i=1}^{N^2-1} c_{iN^2}\hat{\mathsf{F}}_i, \\ \hat{\mathsf{G}} &= \frac{1}{2N}a_{N^2N^2}\mathbb{1}_{\mathrm{S}} + \frac{1}{2}\left(\hat{\mathsf{F}}+\hat{\mathsf{F}}^\dagger\right), \\ \hat{\mathsf{H}} &= \frac{\mathrm{i}\hbar}{2}\left(\hat{\mathsf{F}}-\hat{\mathsf{F}}^\dagger\right), \end{aligned} \tag{B.7}$$

and gives

$$\mathcal{L}[\rho] = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}},\rho\right] + \left\{\hat{\mathsf{G}},\rho\right\} + \sum_{i,j}^{N^2-1} a_{ij}\hat{\mathsf{F}}_i\rho\hat{\mathsf{F}}_j^\dagger. \tag{B.8}$$

The fact that the semigroup mapping $\mathcal{M}_t$ is trace preserving, implies that the generator has a vanishing trace,

$$0 = \mathrm{Tr}\left[\mathcal{L}[\rho]\right] = \mathrm{Tr}\left[\left(2\hat{\mathsf{G}} + \sum_{i,j}^{N^2-1} a_{ij}\hat{\mathsf{F}}_j^\dagger\hat{\mathsf{F}}_i\right)\rho\right], \tag{B.9}$$

where I used the cyclic invariance of the trace in the second equation. Since Eq. (B.9) must hold for all density matrices ρ one gets the condition

$$\hat{\mathsf{G}} = -\frac{1}{2}\sum_{i,j}^{N^2-1} a_{ij}\hat{\mathsf{F}}_j^\dagger\hat{\mathsf{F}}_i, \tag{B.10}$$

which gives rise to the *first standard form* of the generator,

$$\mathcal{L}[\rho] = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}},\rho\right] + \sum_{i,j}^{N^2-1} a_{ij}\left(\hat{\mathsf{F}}_i\rho\hat{\mathsf{F}}_j^\dagger - \frac{1}{2}\left\{\hat{\mathsf{F}}_j^\dagger\hat{\mathsf{F}}_i,\rho\right\}\right). \tag{B.11}$$

If the $\hat{\mathsf{F}}_i$ are chosen dimensionless, one deduces from Eqs. (B.4) and (B.7) that the c_{ij} and therefore the a_{ij} have the dimension of a frequency and that $\hat{\mathsf{H}}$ has the dimension of an energy. Moreover, the matrix c_{ij} is positive as for every vector $\boldsymbol{v}\in\mathbb{C}^{N^2}$

$$\begin{aligned} \sum_{i,j} c_{ij}v_i^*v_j &= \sum_{\alpha,\beta}\left(\sum_i v_i\hat{\mathsf{F}}_i, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right)\left(\sum_j v_j\hat{\mathsf{F}}_j, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right)^* \\ &= \sum_{\alpha,\beta}\left|\left(\sum_i v_i\hat{\mathsf{F}}_i, \hat{\mathsf{W}}_{\alpha,\beta}(t)\right)\right|^2 \geq 0. \end{aligned}$$

Accordingly, also the matrix a_{ij} is positive and can be diagonalized via a unitary transformation u,

$$uau^\dagger = \mathrm{diag}\left(\gamma_1, \ldots, \gamma_{N^2-1}\right), \tag{B.12}$$

with non-negative eigenvalues γ_i. One then defines the *Lindblad operators* $\hat{\mathsf{L}}_j$ through

$$\hat{\mathsf{F}}_i = \sum_{j=1}^{N^2-1} u_{ji}\hat{\mathsf{L}}_j, \tag{B.13}$$

and arrives at the diagonal form of the generator (B.11),

$$\mathcal{L}[\rho_\mathrm{S}] = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathsf{H}}, \rho_\mathrm{S}\right] + \sum_{i=1}^{N^2-1}\gamma_i\left(\hat{\mathsf{L}}_i\rho_\mathrm{S}\hat{\mathsf{L}}_i^\dagger - \frac{1}{2}\left\{\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i, \rho_\mathrm{S}\right\}\right). \tag{B.14}$$

The upper limit of the summation in Eq. (B.14) denotes a maximum value and there may as well be less Lindblad operators present.[1] The case presented above of a finite dimensional Hilbert space $\mathcal{H}_\mathrm{S}$ has been treated by Gorini, Kossakowski and Sudarshan [52] whereas Lindblad [51] showed the derivation of Eq. (B.14) for an infinite dimensional Hilbert space where i runs over a countable set and the Lindblad operators being bounded. However, for unbounded operators there is no such general statement about the form of the generator $\mathcal{L}$, although all known semigroup generators can be brought into the above form (B.14). For example, in the case of quantum Brownian motion as treated in Chapter 4, one has unbounded Lindblad operators being a linear compination of the position and momentum operators.

B.2. Derivation of the nonlinear pointer state equation

As stated in Section 3.6.1, the NLPSE is obtained by looking for an evolution equation for pure states, $\hat{\mathsf{P}} = |\psi\rangle\langle\psi| = \hat{\mathsf{P}}^2$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathsf{P}} = \hat{\mathsf{N}}[\hat{\mathsf{P}}], \tag{B.15}$$

which is closest to the density matrix evolution of the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathcal{L}[\rho]. \tag{B.16}$$

Here, $\hat{\mathsf{N}}[\cdot]$ is a nonlinear operator and $\mathcal{L}[\cdot]$ the generator of the master equation, which is not necessarily of the Lindblad form (3.39). The above statement can be formulated as an optimization problem of minimizing the Hilbert-Schmidt norm

$$\min_{\hat{\mathsf{N}}[\hat{\mathsf{P}}]}\left\|\mathcal{L}[\hat{\mathsf{P}}] - \hat{\mathsf{N}}[\hat{\mathsf{P}}]\right\|_\mathrm{HS}^2 \tag{B.17}$$

[1] For a set of N' Lindblad operators one sets $\gamma_i = 0$ for $N^2 - 1 \geq i > N'$.

over all possible pure state evolutions described by $\hat{\mathsf{N}}\left[\hat{\mathsf{P}}\right]$. The Hilbert-Schmidt norm of an operator $\hat{\mathsf{A}}$ is defined as

$$\left\|\hat{\mathsf{A}}\right\|_{\mathrm{HS}}^2 \equiv \mathrm{Tr}\left[\hat{\mathsf{A}}^\dagger\hat{\mathsf{A}}\right]. \tag{B.18}$$

Before solving the minimization problem (B.17), I rewrite the nonlinear operator by using that the pure state evolution (B.15) is norm preserving and that it maps pure states to pure states. At first, for a completely general pure state evolution one can make the decomposition

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \left(\hat{\mathsf{A}}'_\psi + \hat{\mathsf{B}}_\psi\right)|\psi\rangle, \tag{B.19}$$

into a hermitian and an anti-hermitian part, $\hat{\mathsf{A}}'_\psi = \hat{\mathsf{A}}'^\dagger_\psi$ and $\hat{\mathsf{B}}_\psi = -\hat{\mathsf{B}}^\dagger_\psi$, with $\hat{\mathsf{A}}'_\psi$ and $\hat{\mathsf{B}}_\psi$ being state-dependent. The preservation of the norm together with Eq. (B.19) implies

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle = 2\langle\hat{\mathsf{A}}'_\psi\rangle, \tag{B.20}$$

with expectation value $\langle\hat{\mathsf{A}}'_\psi\rangle = \langle\psi|\hat{\mathsf{A}}'_\psi|\psi\rangle$. Thus, by setting

$$\hat{\mathsf{A}}'_\psi = \hat{\mathsf{A}}_\psi - \langle\hat{\mathsf{A}}_\psi\rangle, \tag{B.21}$$

with hermitian operator $\hat{\mathsf{A}}_\psi$, Eq. (B.19) is norm preserving.

In a next step, I deduce the corresponding form of Eq. (B.19) for the projector $\hat{\mathsf{P}} = |\psi\rangle\langle\psi| = \hat{\mathsf{P}}^2$. One calculates

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathsf{P}} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi\rangle\langle\psi|\right)\\ &= \left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\hat{\mathsf{A}}_\psi\right]\right] + \left[\hat{\mathsf{B}}_\psi,\hat{\mathsf{P}}\right]\\ &= \left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\hat{\mathsf{A}}_\psi + \left[\hat{\mathsf{B}}_\psi,\hat{\mathsf{P}}\right]\right]\right],\end{aligned} \tag{B.22}$$

where it is used that

$$\begin{aligned}\left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\hat{\mathsf{A}}_\psi\right]\right] &= \hat{\mathsf{P}}^2\hat{\mathsf{A}}_\psi + \hat{\mathsf{A}}_\psi\hat{\mathsf{P}}^2 - \hat{\mathsf{P}}\hat{\mathsf{A}}_\psi\hat{\mathsf{P}}\\ &= \hat{\mathsf{P}}\left(\hat{\mathsf{A}}_\psi - \hat{\mathsf{A}}_\psi\hat{\mathsf{P}}\right) + \left(\hat{\mathsf{A}}_\psi - \hat{\mathsf{P}}\hat{\mathsf{A}}_\psi\right)\hat{\mathsf{P}},\end{aligned} \tag{B.23}$$

and $\langle\hat{\mathsf{A}}_\psi\rangle\hat{\mathsf{P}} = \hat{\mathsf{P}}\hat{\mathsf{A}}_\psi\hat{\mathsf{P}}$. Thus, according to Eq. (B.22), any trace preserving equation for pure states can be written in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathsf{P}} = \left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\hat{\mathsf{C}}_\psi\right]\right] = \hat{\mathsf{N}}[\hat{\mathsf{P}}], \tag{B.24}$$

where I introduced the hermitian state-dependent operator $\hat{\mathsf{C}}_\psi = \hat{\mathsf{A}}_\psi + \left[\hat{\mathsf{B}}_\psi,\hat{\mathsf{P}}\right]$.

The optimization problem (B.17) over all $\hat{\mathsf{N}}\left[\hat{\mathsf{P}}\right]$ reformulates to finding a hermitian $\hat{\mathsf{C}}_\psi$ that minimizes the Hilbert-Schmidt distance. Plugging expression (B.24) for the nonlinear operator $\hat{\mathsf{N}}[\hat{\mathsf{P}}]$ into Eq. (B.17), one gets

$$\begin{aligned}\left\|\mathcal{L}[\hat{\mathsf{P}}]-\hat{\mathsf{N}}[\hat{\mathsf{P}}]\right\|_{\mathrm{HS}}^2 &= \mathrm{Tr}\left[\left(\mathcal{L}[\hat{\mathsf{P}}]-\left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\hat{\mathsf{C}}_\psi\right]\right]\right)^2\right]\\ &= \mathrm{Tr}\left[\mathcal{L}[\hat{\mathsf{P}}]^2-2\left(\mathcal{L}[\hat{\mathsf{P}}]^2\hat{\mathsf{P}}-\left(\mathcal{L}[\hat{\mathsf{P}}]\hat{\mathsf{P}}\right)^2\right)\right]\\ &\quad+2\mathrm{Tr}\left[\left(\mathcal{L}[\hat{\mathsf{P}}]-\hat{\mathsf{C}}_\psi\right)^2\hat{\mathsf{P}}-\left(\left(\mathcal{L}[\hat{\mathsf{P}}]-\hat{\mathsf{C}}_\psi\right)\hat{\mathsf{P}}\right)^2\right],\end{aligned} \tag{B.25}$$

where one makes extensive use of the projector property $\hat{\mathsf{P}}=\hat{\mathsf{P}}^2$ and the cyclic invariance of the trace $\mathrm{Tr}\left[\hat{\mathsf{X}}\hat{\mathsf{Y}}\right]=\mathrm{Tr}\left[\hat{\mathsf{Y}}\hat{\mathsf{X}}\right]$. The first summand of Eq. (B.25) is independent of $\hat{\mathsf{C}}_\psi$ and therefore does not take part in the minimization procedure; the second summand can be further rewritten by introducing $\hat{\mathsf{D}}_\psi=\mathcal{L}[\hat{\mathsf{P}}]-\hat{\mathsf{C}}_\psi$ so that the term to minimize reads

$$2\mathrm{Tr}\left(\hat{\mathsf{D}}_\psi^2\hat{\mathsf{P}}-\hat{\mathsf{D}}_\psi\hat{\mathsf{P}}\hat{\mathsf{D}}_\psi\hat{\mathsf{P}}\right)=2\left(\langle\hat{\mathsf{D}}_\psi^2\rangle-\langle\hat{\mathsf{D}}_\psi\rangle^2\right). \tag{B.26}$$

But this is nothing else than the definition of the variance of $\hat{\mathsf{D}}_\psi$. The variance vanishes and thus is minimized for eigenstates $\hat{\mathsf{D}}_\psi|\psi\rangle=\lambda|\psi\rangle$, which implies $\hat{\mathsf{C}}_\psi\hat{\mathsf{P}}=\left(\mathcal{L}[\hat{\mathsf{P}}]-\lambda\right)\hat{\mathsf{P}}$. With Eq. (B.24) one finally arrives at [21]

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathsf{P}}=\left[\hat{\mathsf{P}},\left[\hat{\mathsf{P}},\mathcal{L}[\hat{\mathsf{P}}]\right]\right]. \tag{B.27}$$

The form I will use throughout this work is the corresponding equivalent state vector equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle=\left(\mathcal{L}[\hat{\mathsf{P}}]-\langle\mathcal{L}[\hat{\mathsf{P}}]\rangle\right)|\psi\rangle. \tag{B.28}$$

For generators $\mathcal{L}[\cdot]$ of Lindblad master equations, see Eq. (3.39), the nonlinear pointer state equation takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle=\hat{\mathsf{N}}\left[\psi\right]|\psi\rangle=\left[\frac{1}{\mathrm{i}\hbar}\left(\hat{\mathsf{H}}-\overline{H}\right)+\sum_i\left(\frac{1}{2}\left(\overline{L_i^\dagger L_i}-\hat{\mathsf{L}}_i^\dagger\hat{\mathsf{L}}_i\right)+\overline{L_i^\dagger}\left(\hat{\mathsf{L}}_i-\overline{L}_i\right)\right)\right]|\psi\rangle, \tag{B.29}$$

with Hamiltonian $\hat{\mathsf{H}}$ and Lindblad operators $\hat{\mathsf{L}}_i$. Note that the rates γ_i are absorbed into the Lindblad operators, in this representation.

C. Quantum Brownian motion

C.1. Stability of the fixed points of the variances

The stability of the pointer state variances is checked by considering small deviations around the fixed points

$$\begin{aligned} V_x &= V_{x,\mathrm{ps}} + \varepsilon_x, \\ C_{xp} &= C_{xp,\mathrm{ps}} + \varepsilon_{xp}, \end{aligned} \tag{C.1}$$

where $V_{x,\mathrm{ps}}$ and $C_{xp,\mathrm{ps}}$ are given in Eqs. (4.5). Equations (C.1) are inserted into the corresponding differential equations (4.3) and expanded to first order in the deviations ε_x and ε_{xp}. One gets the linearized differential equations

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_x &= \varepsilon_x \left(1 - 8\kappa^2 V_{x,\mathrm{ps}}\right) + \varepsilon_{xp}\left(1 - \frac{C_{xp,\mathrm{ps}}}{8}\right), \\ \frac{\mathrm{d}}{\mathrm{d}t}\varepsilon_{xp} &= -\varepsilon_x 8\kappa^2 C_{xp,\mathrm{ps}} - \varepsilon_{xp}\left(1 + \frac{1 + \kappa^2 C_{xp,\mathrm{ps}}^2}{8\kappa^2 V_{x,\mathrm{ps}}}\right), \end{aligned} \tag{C.2}$$

which can be cast into the matrix form $\mathrm{d}\boldsymbol{\varepsilon}/\mathrm{d}t = \mathsf{M}\boldsymbol{\varepsilon}$. The deviations $\boldsymbol{\varepsilon}$ decay exponentially if the matrix M has only negative eigenvalues. The two eigenvalues of M are

$$\lambda_{1,2} = -y \pm \sqrt{y^2 + \frac{1 + \kappa^2 C_{xp,\mathrm{ps}}^2 - 64\kappa^4 V_{x,\mathrm{ps}}\left(C_{xp,\mathrm{ps}} + V_{x,\mathrm{ps}}\right)}{8\kappa^2 V_{x,\mathrm{ps}}}}, \tag{C.3}$$

with the abbreviation

$$y = \frac{1 + \kappa^2 C_{xp,\mathrm{ps}}^2 + 64\kappa^4 V_{x,\mathrm{ps}}^2}{16\kappa^2 V_{x,\mathrm{ps}}}. \tag{C.4}$$

The negativity of the eigenvalues reduces to the condition

$$1 + \kappa^2 C_{xp,\mathrm{ps}}^2 - 64\kappa^4 V_{x,\mathrm{ps}}\left(C_{xp,\mathrm{ps}} + V_{x,\mathrm{ps}}\right) < 0, \tag{C.5}$$

which can be confirmed easily by plotting the term. In conclusion, small deviations from $V_{x,\mathrm{ps}}$ and $C_{xp,\mathrm{ps}}$ decay exponentially and render them stable fixed points.

C.2. Stability of a single wave packet in a superposition

The weight equations in (4.13) describe the time evolution of the individual weights of the constituents of the superposition state (4.7). They exhibit stable fixed points if one

weight equals unity while the others vanish; without loss of generality let us assume that $w_1 = 1$ and $w_j = 0$ for $j \in \{2, \ldots, N\}$.

The equation of motion for w_1 then reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}w_1 &= w_1\left(2\kappa^2\left(V_x - V_{x,1} - (\overline{x} - \overline{x}_1)^2\right) + \frac{1}{8}\left(V_p - V_{p,1} - (\overline{p} - \overline{p}_1)^2\right)\right) \\ &= -\sum_{j=1}^{N} w_j F_{1j} + \sum_{j,k=1}^{N} w_j w_k F_{jk},\end{aligned} \tag{C.6}$$

with the definition

$$F_{jk} = 2\kappa^2\left(V_{x,j} + V_{x,k} + (\overline{x}_j - \overline{x}_k)^2\right) + \frac{1}{8}\left(V_{p,j} + V_{p,k} + \left(\overline{p}_j - \overline{p}_k\right)^2\right). \tag{C.7}$$

Small perturbations from the fixed point are accounted for by setting

$$w_1 = 1 - \varepsilon, \tag{C.8}$$

and maintaining the normalization condition $\sum_{j=1}^{N} w_j = 1$. This requires that, for $j \neq 1$,

$$w_j = \mathcal{O}(\varepsilon), \tag{C.9}$$

i.e. these weights are at least of order ε. Using Eq. (C.8), one gets from the temporal evolution of w_1

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon &= (1-\varepsilon)\left(\sum_{j=1}^{N} w_j F_{1j} - \sum_{j,k=1}^{N} w_j w_k F_{jk}\right) \\ &= (1-\varepsilon)\left[w_1 F_{11} + \sum_{j=2}^{N} w_j F_{1j} - \left(w_1^2 F_{11} + 2w_1 \sum_{j=2}^{N} w_j F_{1j} + \sum_{j,k=2}^{N} w_j w_k F_{jk}\right)\right] \\ &= \varepsilon F_{11} - \sum_{j=2}^{N} w_j F_{1j},\end{aligned} \tag{C.10}$$

where it is used that $F_{jk} = F_{kj}$ and only terms to order ε are kept. In the situation considered here, namely, for wave packet separations much larger than the width of each wave packet, the off-diagonals F_{1j} are much larger than the diagonal F_{11}. It follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\varepsilon < 0, \tag{C.11}$$

which leads to an exponential decay of small perturbations around the fixed point and confirms its stability.

C.3. Correlation between the subpeaks in phase space after a jump

According to Eq. (4.31), the wave function after a jump has a double-peaked structure,

$$\psi'(x) = \mathcal{N}_1 \left(x - \overline{x}\right) \pi_{\overline{x},\overline{p}}\left(x\right), \tag{C.12}$$

with normalizing factor

$$\mathcal{N}_1 = \sqrt{\frac{2}{r_{\mathrm{ps}}}}\kappa \left(1 - \frac{1 - \mathrm{i}\kappa C_{xp,\mathrm{ps}}}{8\kappa^2 V_{x,\mathrm{ps}}}\right), \tag{C.13}$$

leading to $1 = |\mathcal{N}_1|^2 V_{x,\mathrm{ps}}$. The suppression of one subpeak by the NLPSE is approximately accounted for by cutting it away and renormalizing the state. In particular, suppression of the left subpeak in Eq. (C.12) yields

$$\psi''(x) = \sqrt{2}\Theta\left(x - \overline{x}\right)\psi'(x), \tag{C.14}$$

where the factor $\sqrt{2}$ keeps the function normalized and $\Theta\left(\cdot\right)$ denotes the Heaviside step function. Clearly, for the position expectation one gets $\overline{x}'' > \overline{x}$ because $\psi''(x)$ vanishes for $x < \overline{x}$. For the momentum expectation, one calculates

$$\begin{aligned}
\overline{p}'' &= \langle\psi''|\hat{\mathsf{p}}|\psi''\rangle \\
&= \int \mathrm{d}x \psi''^{*}(x) \left(-\frac{\mathrm{i}}{\kappa}\right) \frac{\partial}{\partial x}\psi''(x) \\
&= 2\left|\mathcal{N}_1\right|^2 \int_{\overline{x}}^{\infty} \mathrm{d}x \left(-\frac{\mathrm{i}}{\kappa}\left(x - \overline{x}\right) + \overline{p}\left(x - \overline{x}\right)^2 + \frac{\mathrm{i}/\kappa + C_{xp,\mathrm{ps}}}{2V_{x,\mathrm{ps}}}\left(x - \overline{x}\right)^3\right) \left|\pi_{\overline{x},\overline{p}}(x)\right|^2 \\
&= \overline{p} + \frac{C_{xp,\mathrm{ps}}}{\sqrt{2\pi V_{x,\mathrm{ps}}}},
\end{aligned} \tag{C.15}$$

where in the third line, one calculates the integrals by using that the pointer state is Gaussian. Since the covariance $C_{xp,\mathrm{ps}}$ of the pointer state, which is shown in Eq. (4.5), is positive, one infers that $\overline{p}'' > \overline{p}$. The argument goes exactly along the same steps if the right subpeak was suppressed. This leads to the finding that both in position and momentum representation always the same subpeak survives.

D. Quantum linear Boltzmann equation

D.1. Useful relations for the momentum integrals

The QLBE (6.1) involves the integration of the Lindblad operators (6.3) over all momentum transfers $\boldsymbol{Q}$ and over momenta $\boldsymbol{k}_\perp$ perpendicular to $\boldsymbol{Q}$. If the integrand exhibits certain symmetries, these integrations can be simplified substantially. I will collect here the calculations that lead to useful simplifications:

1.
$$\int\limits_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \, g\left(k_\perp, \boldsymbol{Q}\right) = 2\pi \int\limits_0^\infty \mathrm{d}k \, k \, g\left(k, \boldsymbol{Q}\right), \tag{D.1}$$

with $g\left(k_\perp, \boldsymbol{Q}\right)$ being an arbitrary function. The $\boldsymbol{k}_\perp$-integral on the left-hand side goes over the plane perpendicular to $\boldsymbol{Q}$ and thus depends on $\boldsymbol{Q}$, in general. However, the integrand depends on the absolute value $k_\perp$ only, which makes the integral independent of $\boldsymbol{Q}$. This is readily seen by going to polar coordinates.

2.
$$\int\limits_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \, g\left(k_\perp, \boldsymbol{Q}\right) \boldsymbol{k}_\perp \cdot \boldsymbol{P} = 0 \tag{D.2}$$

The scalar product can be written

$$\boldsymbol{k}_\perp \cdot \boldsymbol{P} = \boldsymbol{k}_\perp \cdot \boldsymbol{P}_\perp = k_\perp P_\perp \cos\left(\varphi\right), \tag{D.3}$$

where the vector $\boldsymbol{P}_\perp$ also lies in the plane perpendicular to $\boldsymbol{Q}$ and I used polar coordinates with abcsissa going in $\boldsymbol{P}_\perp$-direction. Integration over the polar angle φ then gives the above result.

3.
$$\int\limits_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \, g\left(k_\perp, \boldsymbol{Q}\right) \frac{\left(\boldsymbol{k}_\perp \cdot \boldsymbol{P}\right)\left(\boldsymbol{k}_\perp \cdot \boldsymbol{R}\right)}{k_\perp^2} = \frac{1}{2} \int\limits_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp \, g\left(k_\perp, \boldsymbol{Q}\right) \left(\boldsymbol{P} \cdot \boldsymbol{R} - \frac{\left(\boldsymbol{Q} \cdot \boldsymbol{P}\right)\left(\boldsymbol{Q} \cdot \boldsymbol{R}\right)}{Q^2} \right) \tag{D.4}$$

Similar to the previous derivation, one uses polar coordinates with abcsissa in $\boldsymbol{P}_\perp$-direction. The two scalar products on the left-hand side are then rewritten,

$$(\boldsymbol{k}_\perp \cdot \boldsymbol{P})(\boldsymbol{k}_\perp \cdot \boldsymbol{R}) = (\boldsymbol{k}_\perp \cdot \boldsymbol{P}_\perp)(\boldsymbol{k}_\perp \cdot \boldsymbol{R}_\perp) = k_\perp^2 P_\perp R_\perp \cos(\varphi)\left[\cos(\varphi)\cos(\delta) + \sin(\varphi)\sin(\delta)\right], \quad \text{(D.5)}$$

with the angles $\varphi = \angle(\boldsymbol{k}_\perp, \boldsymbol{P}_\perp)$ and $\delta = \angle(\boldsymbol{P}_\perp, \boldsymbol{R}_\perp)$. Finally, the integral to calculate reads

$$\int_0^\infty \mathrm{d}k\, k \int_0^{2\pi} \mathrm{d}\varphi\, g(k, \boldsymbol{Q})\, P_\perp R_\perp \left(\cos^2(\varphi)\cos(\delta) + \frac{1}{2}\sin(2\varphi)\sin(\delta)\right), \quad \text{(D.6)}$$

where $2\sin(\varphi)\cos(\varphi) = \sin(2\varphi)$ is used. The second summand vanishes upon the φ-integration, whereas the first summand gives

$$\int_0^{2\pi} \mathrm{d}\varphi \cos^2(\varphi) = \frac{1}{2}\int_0^{2\pi} \mathrm{d}\varphi. \quad \text{(D.7)}$$

The form of Eq. (D.4) is obtained by using that the perpendicular component of any vector can be written $\boldsymbol{A}_\perp = \boldsymbol{A} \cdot \left(\mathbb{1} - \boldsymbol{Q} \otimes \boldsymbol{Q}/Q^2\right)$. Rewriting $\boldsymbol{P}_\perp$ and $\boldsymbol{R}_\perp$ then yields

$$\begin{aligned} P_\perp R_\perp \cos(\delta) &= \boldsymbol{P}_\perp \cdot \boldsymbol{R}_\perp = \boldsymbol{P} \cdot \left(\mathbb{1} - \frac{\boldsymbol{Q} \otimes \boldsymbol{Q}}{Q^2}\right)^2 \cdot \boldsymbol{R} \\ &= \boldsymbol{P} \cdot \left(\mathbb{1} - \frac{\boldsymbol{Q} \otimes \boldsymbol{Q}}{Q^2}\right) \cdot \boldsymbol{R} = \boldsymbol{P} \cdot \boldsymbol{R} - \frac{(\boldsymbol{Q} \cdot \boldsymbol{P})(\boldsymbol{Q} \cdot \boldsymbol{R})}{Q^2}. \end{aligned} \quad \text{(D.8)}$$

4.

$$\int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}_\perp} \mathrm{d}\boldsymbol{k}_\perp\, g(k_\perp, Q)\, Q_i^{2n+1} = 0 \quad \text{(D.9)}$$

Notice that the function $g(k_\perp, Q)$ now depends on the absolute value Q only. From Eq. (D.1), we already know that the $\boldsymbol{k}_\perp$-integral is independent of $\boldsymbol{Q}$. Moreover, the absolute value $Q = \sqrt{\sum_j Q_j^2}$ is an even function in the cartesian components of $\boldsymbol{Q}$, hence the whole integrand is odd in Q_i and the integral vanishes. This argument naturally generalizes to any function g being even in every cartesian component of $\boldsymbol{Q}$.

Introducing the notation "$a \cong b$", which means that "a equals b below the $\boldsymbol{k}_\perp$- and $\boldsymbol{Q}$- integrals", one can put the above relations into a shortened form. Equation (D.2) becomes

$$g(k_\perp, \boldsymbol{Q})\, \boldsymbol{k}_\perp \cong 0. \quad \text{(D.10)}$$

Equation (D.4) can be rewritten using the dyadic product and one gets

$$g\left(k_{\perp}, \boldsymbol{Q}\right) \frac{\boldsymbol{k}_{\perp} \otimes \boldsymbol{k}_{\perp}}{k_{\perp}^{2}} \cong \frac{1}{2} g\left(k_{\perp}, \boldsymbol{Q}\right) \left(\mathbb{1} - \frac{\boldsymbol{Q} \otimes \boldsymbol{Q}}{Q^{2}}\right). \tag{D.11}$$

The integral relation involving odd powers of Q_j, see Eq. (D.9), is now simply expressed as

$$g\left(k_{\perp}, Q\right) Q_{j}^{2n+1} \cong 0. \tag{D.12}$$

This means, in particular, that the integral involving the vector $\boldsymbol{Q}$ also vanishes,

$$g\left(k_{\perp}, Q\right) \boldsymbol{Q} \cong 0. \tag{D.13}$$

Additionally, relations like

$$g\left(k_{\perp}, Q\right) Q_{j}^{2n+1} Q_{k}^{2m} \cong 0 \tag{D.14}$$

are readily derived by the above reasoning. Finally, since $Q = \sqrt{\sum_j Q_j^2}$ is not only even but also symmetric with respect to the cartesian components Q_j, one can arrive at the useful form

$$g\left(k_{\perp}, Q\right) Q_{j} Q_{k} \cong \delta_{jk} g\left(k_{\perp} Q\right) \frac{Q^{2}}{3}. \tag{D.15}$$

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